IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

Applicant:

Jonathan Scott Brecher

Serial No.:

To Be Assigned

Filed:

Herewith (This application claims the benefit of U.S. Provisional Application Serial No.

60/119,930 entitled DERIVING A CHEMICAL STRUCTURE FROM A

CHEMICAL NAME, filed on February 12, 1999.)

Title:

DERIVING CHEMICAL STRUCTURAL INFORMATION

Box Patent Application Assistant Commissioner for Patents Washington, DC 20231

COVER SHEET FOR APPENDIX: NOMTOKENS

Dear Sir:

Enclosed for filing in the above-referenced patent application is the following document:

1. Appendix: NOMTOKENS, 111 pages.

The following is the inventor's residence: 52 Montgomery Street, #2, Cambridge, MA 02140.

Respectfully submitted,

Dated: February 11, 2000

Jason A. Reyes

Registration No. 41,513 Attorney for Applicant

Hale and Dorr LLP 60 State Street Boston, MA 02109

Tel.: (617) 526-6010

Fax: (617) 526-5000

EXPRESS MAIL LABEL NO. EM259723548US

Attorney Docket No. 103544.127 DATE OF DEPOSIT February 11, 2000

```
meth|carbin root alkane C,a|alpha|1|w|omega
carbenium root root [C+],1|w|omega
carbene root root C,32@1|w|omega
aminylene nitrene root root N,32@1 | w | omega
hydroxymethyl root root C,40x,0,x
hydroxymethylene root root C,8@x,0,x
form root trivial C, x | 1 | w | omega, (=0), x
formimino root trivial C,4@x | 1 | w | omega, (=N), x
formalin root root C=0,x
eth root alkane C,1|a|alpha,C,2|b|beta|w|omega
ethene|ethen root alkane C,1|a|alpha,=,x,C,2|b|beta|w|omega
ethyne|ethyn root alkane C,1|a|alpha,#,x,C,2|b|beta|w|omega
acet root trivial C,1, (=,x,0,x,),x,C,2|a|alpha|w|omega
aceto root trivial C,401, (=,x,0,x,),x,C,2|a|alpha|w|omega
acetoacet acetoaceto root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3,(=,x,0,x,),x,C,4|g|gamma|w|omega|
prop|propa root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma|w|omega
isoprop|isopropa|isopropion root alkane C,a|alpha,(,x,C,b|beta,),x,C,x
hexafluoroisoprop|hexafluoroisopropa root alkane
C,a|alpha,(C(F)(F)F),x,C(F)(F)F,x
propiono | propion | propio | propi root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta|w|omega
proparg|proparag root alkane C,1|a|alpha,C,2,#,x,C,3|w|omega
tetrol loveracid alkane C,1,C,2,#,x,C,3,C,4|w|omega
butyro|butyr root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma|w|omega
isobutyro isobutyr root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,4|b'|beta'|g|gamma|w|omega|
isobutylene root root C=C(C)C,x
crotono croton root trivial
C,1,(=,x,0,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
\texttt{crot root C,1,/,x,C,2} \\ | \texttt{a}| \\ \texttt{alpha,=,x,C,3} \\ | \texttt{b}| \\ \texttt{beta,/,x,C,4} \\ | \texttt{g}| \\ \texttt{gamma} \\ | \texttt{w}| \\ \texttt{omega} \\ | \texttt{omega}| \\ \texttt{omega}
crotonylalcohol root root
C,1,(0),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
isocrotono isocroton root trivial
C,1, (=,x,0,x,),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega|
isocrot root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega|
seneci root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,=,x,C,3|b|beta,(,x,C,4|g|gamma|w|omega,),x,C,4'|g'|
gamma' w' omega'
tigl|cevad root trivial
C,1,(=,x,0,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega|
angel root trivial
C,1,(=,x,0,x,),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega|
pren root alkane C,1,C,2|a|alpha,=,x,C,3|b|beta,(C),x,C,4|g|gamma|w|omega
valero|valer|valerian root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
acetonoxal root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(=0),x,C,3|b|beta,C,4|g|gamma,(=0),x,C,5|d|delta|w|
omega
 valpr root trivial
\texttt{C,1,(=,x,0,x,),x,C,2} \\ \texttt{|alpha,(CCC),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega}
 levulin|laevulin|levul root trivial
 C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4,(=0),x,C,5|g|gamma|d|delta|w|omega|
 isovalero|isovaler|delphin root trivial
  \texttt{C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,(,x,C,4|g|gamma,),x,C,5|d|delta|w|omega} \\
```

```
pival root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(,x,C,3|b|beta,)(,x,C,4|3',),x,C,5|3''
amyl root alkane C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
capro root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon|w|omega
acexam root root
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=0),x,
enatho|enanth|oenantho|oenanth root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7|w|omega
geron root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(C)(C),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6|e|e|a|delta,C,6
psilon, (=0), x, C, 7 | w | omega
capryl root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8|w|omega
octoate root root
0,10x,C,1,(=0),x,C,2|a|alpha,(,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilo
n,),x,C,x,C,x
pelargono|pelargon|pelarg|pergon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9|w|o
capr root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|q|qamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0 w omega
obtusil root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10|w|omega
stilling root alkane
C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma,=,x,C,5|d|delta,\,x,C,6|e|eps
ilon, C, 7, C, 8, C, 9, C, 10 | w | omega
lauro|laur|vulv|laurostear root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12|w|omega
linder root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12|w|omega
myristo myrist root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14|w|omega
physeter|physoter root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,=,x,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12,C,13,C,14|w|omega
ipurol root alkane
C,1,C,2|a|alpha,C,3|b|beta,(0),x,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,(0),x,C,12,C,13,C,14|w|omega
tsuzu tudu root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
,C,10,C,11,C,12,C,13,C,14|w|omega
myristelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
= x, C, 10, /, x, C, 11, C, 12, C, 13, C, 14 | w | omega
myristole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
= x, C, 10, x, C, 11, C, 12, C, 13, C, 14 | w | omega
palmito|palmit|cet root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
```

```
palmitelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
palmitole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
, = , x, C, 10, \ x, C, 11, C, 12, C, 13, C, 14, C, 15, C, 16 \ w \ omega
hiragon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,=,x,C,7,C,8,C,9
,C,10,=,x,C,11,C,12,C,13,C,14,=,x,C,15,C,16|w|omega
ustil root alkane
C,1,C,2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,C,12,C,13,C,14,C,15,(0),x,C,16|w|omega,O,x
ambrettol root alkane
\texttt{C,1,C,2} \\ \texttt{|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,=,x,C} \\ \texttt{|c,1,C,2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,=,x,C} \\ \texttt{|c,1,C,2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta,C,5|d|delta
,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,0,x
aleurit root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(0)
, x, C, 10, (0), x, C, 11, C, 12, C, 13, C, 14, C, 15, C, 16 |w| omega, 0, x
gaid|hypogae root alkane
C,1,C,2|a|alpha,=,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega
juniper root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0, C, 11, C, 12, C, 13, C, 14, C, 15, C, 16 | w | omega, 0, x
margaro | margar root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17|w|omega
stear stearophan root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
moroct root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,=,x
 ,C,9,C,10,C,11,C,12,=,x,C,13,C,14,C,15,=,x,C,16,C,17,C,18|w|omega
parinar root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,=,x
 ,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,=,x,C,16,C,17,C,18|w|omega
 eleostear root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 = x, C, 10, x, C, 11, = x, C, 12, x, C, 13, = x, C, 14, x, C, 15, C, 16, C, 17, C, 18 | w | omega
 stearol loveracid root
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,\#,x
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 couep lican root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,(=0),x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,
 C, 9, =, x, C, 10, C, 11, =, x, C, 12, C, 13, =, x, C, 14, C, 15, C, 16, C, 17, C, 18 | w | omega
 trichosan root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 = x, C, 10, /, x, C, 11, =, x, C, 12, /, x, C, 13, =, x, C, 14, /, x, C, 15, C, 16, C, 17, C, 18 | w | omega
 floionol phloionol root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(0)
 ,x,C,10,(0),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega,0,x
 lycaon root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,(=0),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 lactarin root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=0),x,C,7,C,8,
 C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
```

```
jalapinol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,(0),x,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
ole root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
elaid root alkane
C.1,C.2|a|alpha,C.3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
ricinole ricinol root alkane
c,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 , = , x, C, 10, \, x, C, 11, [C@H], 12, (O), x, C, 13, C, 14, C, 15, C, 16, C, 17, C, 18 | w | omega
ricinelaid root alkane
,=,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
linole|telfair root alkane
\texttt{C,1,C,2} \\ | \textbf{a}| \textbf{alpha,C,3} \\ | \textbf{b}| \textbf{beta,C,4} \\ | \textbf{g}| \textbf{gamma,C,5} \\ | \textbf{d}| \textbf{delta,C,6} \\ | \textbf{e}| \textbf{epsilon,C,7,C,8,/,x,C,9} \\ | \textbf{e}| \textbf{epsilon,C,7,C,8,//,x,C,9} \\ | \textbf{epsilon,C,7,C,9,//,x,C,9} \\ | \textbf{epsilon,C,7,C,9,//,x,C,9,//,x,C,9,
 =, x, C, 10, \, x, C, 11, /, x, C, 12, =, x, C, 13, \, x, C, 14, C, 15, C, 16, C, 17, C, 18 | w | omega
vernol loveracid root CCCCCCCC\C=C/C[C@H]1[C@@H](CCCCC)01,x
linolelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 linolenelaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,/,x,C,12,=,x,C,13,/,x,C,14,/,x,C,15,=,x,C,16,/,x,C,17,C,18|w|
linolen alphalinolen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,/,x,C,12,=,x,C,13,\,x,C,14,/,x,C,15,=,x,C,16,\,x,C,17,C,18|w|
gammalinolen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,\,x
 ,C,8,/,x,C,9,=,x,C,10,\setminus,x,C,11,/,x,C,12,=,x,C,13,\setminus,x,C,14,C,15,C,16,C,17,C,18|w|
omega
vaccen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,/,x,C,11,=,x,C,12,/,x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
petroselaid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,=,x,C,7,/,x
 ,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
petroselin root alkane
\texttt{C,1,C,2} \\ | \texttt{alpha,C,3} \\ | \texttt{b|beta,C,4} \\ | \texttt{g|gamma,C,5} \\ | \texttt{d|delta,/,x,C,6} \\ | \texttt{e|epsilon,=,x,C,7,} \\ | \texttt{x,c,c,f} \\ | \texttt{c|epsilon,=,x,C,7,} \\ | \texttt{x,c,c,f} \\ | \texttt{x,c,f} \\ | \texttt{x
 ,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
 calend root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,/,x,C,8,=,x
 \tt,C,9,\backslash,x,C,10,=,x,C,11,\backslash,x,C,12,=,x,C,13,\backslash,x,C,14,C,15,C,16,C,17,C,18|w|omega|
 arachido|arachid|arachin root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
 gadole root alkane
 C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
  ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega
 arachidon root alkane
 C,1,C,2 | a| alpha,C,3 | b| beta,C,4 | g| gamma,/,x,C,5 | d| delta,=,x,C,6 | e| epsilon, \\ \\ \downarrow,x,C,7 | d| delta,=,x,C,6 | e| epsilon,\\ \\ \downarrow,x,C,7 | d| delta,=,x,C,7 | d| delta,=,x,C,7
  ,/,x,C,8,=,x,C,9,\,x,C,10,\/,x,C,11,=,x,C,12,\,x,C,13,\/,x,C,14,=,x,C,15,\,x,C,16,
 C, 17, C, 18, C, 19, C, 20 w omega
```

```
arach root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,c,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21 w omega
lesquerol root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0, /, x, C, 11, =, x, C, 12, \, x, C, 13, [C@H], 14, (0), x, C, 15, C, 16, C, 17, C, 18, C, 19, C, 20, C, 21 | w
omega
beheno behen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,c,11,c,12,c,13,c,14,c,15,c,16,c,17,c,18,c,19,c,20,c,21,c,22 |w|omega
eruc root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w| omeg
brassid root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,/,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22|w| omeg
а
lignocero lignocer root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|omega
cerebron|phrenosin root alkane
C.1.C.2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24|w|
omega
nervon root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,c,11,c,12,c,13,c,14,/,x,c,15,=,x,c,16,\,x,c,17,c,18,c,19,c,20,c,21,c,22,c,23,c
,24 w omega
hyen root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25|w|o
cerotino|cerotin|cerot|cerane root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6 | w | omega
ceryl root alkane
C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C
,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C
,26 | w | omega
cluyt | montano | montan root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6,C,27,C,28|w|omega
melisso|meliss|myric root alkane
0,c,11,c,12,c,13,c,14,c,15,c,16,c,17,c,18,c,19,c,20,c,21,c,22,c,23,c,24,c,25,c,2
6,C,27,C,28,C,29,C,30|w|omega
laccero laccer root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,2
6,C,27,C,28,C,29,C,30,C,31,C,32 w omega
acroleine | acrolein root root C,1,(=,x,0,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
methacrolein root root C,1,(=,x,0,x,),x,C,2|a|alpha,(C),x,=,x,C,3|b|beta|w|omega|
acr root trivial C,1,(=,x,0,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega
hydracr root trivial C,1,(=,x,0,x,),x,C,2,C,3|w| omega,0,0
```

```
methacr root trivial C,1,(=,x,0,x,),x,C,2,(,x,C,4,),x,=,x,C,3|w| omega
propiol root trivial C,1,(=,x,0,x,),x,C,2,\#,x,C,3
glyoxal root trivial C,1,(=,x,0,x,),x,C,2,=,x,0,x
oxalo oxal root diacid C, 1, (=, x, 0, x,), x, C, 402, =, x, 0, x
oxamid oxam root trivial C,1,(=,x,0,x,),x,C,2,(,x,N,n,),x,=,x,0,x
oxanil root trivial
c,1,(=,x,0,x,),x,c,2,(,x,N,n,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
(,), x, =, x, 0, x
mucochlor root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(Cl),x,=,x,C,3|b|beta|w|omega,(Cl),x,C=0,x
mucobrom root trivial
C,1,(=,x,0,x,),x,C,2|a|alpha,(Br),x,=,x,C,3|b|beta|w|omega,(Br),x,C=0,x
pyromuc root root C,x,c,x,Ring,Ring1,c,x,c,x,c,x,o,x,Ring,Ring1
malono malon root diacid C,1,(=,x,0,x,),x,C,2|w| omega,C,4@3,=,x,0,x
tartrono|tartron root diacid C,1,(=,x,0,x,),x,C,2,(,x,0,x,),x,C,403,=,x,0,x
mesoxal root diacid C,1, (=,x,0,x,),x,C,2, (=,x,0,x,),x,C,403,=,x,0,x
mesoxalo root root C,4@1,(=,x,0,x,),x,C,2,(=,x,0,x,),x,C,3,(,x,0,x,),x,=,x,0,x
oxalacet root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3,(=,x,0,x,),x,C,4@4|w|omega,=,x,0,x
oxalaceto root diacid
C.4@1, (=,x,0,x,), x, C.2|a|alpha, C.3, (=,x,0,x,), x, C.4, (,x,0,x,), x,=,x,0,x
succino|succin root diacid C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,404,=,x,0,x
isosuccino isosuccin root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,(,x,C,3|b|beta,),x,C,404,=,x,0,x
caron root diacid
C,1, (=,x,0,x,),x,C,2|a|alpha, (C(C)(C),x,Ring,Ring1,),x,C,3|b|beta,Ring,Ring1,C,4
@4, = , x, 0, x
male | malen | malein | toxil root diacid
C, 1, (=, x, 0, x,), x, /, x, C, 2, =, x, C, 3, \backslash, x, C, 404, =, x, 0, x
fumar|bolet root diacid C,1,(=,x,0,x,),x,/,x,C,2,=,x,C,3,/,x,C,404,=,x,0,x
maleur root trivial C,1, (=,x,0,x,),x,/,x,C,2,=,x,C,3,\,x,C,4,N,x,C,x,(=0),x,N,x
citracon root diacid C,1,(=,x,0,x,),x,/,x,C,2,(C),x,=,x,C,3,\\,x,C,404,=,x,0,x
mesacon root diacid C,1, (=,x,0,x,),x,/,x,C,2,(C),x,=,x,C,3,/,x,C,404,=,x,0,x
teracon root diacid C,1, (=,x,0,x,),x,C,2, (=C(C)C),x,C,3,C,404,=,x,0,x
mal root diacid C,1, (=,x,0,x,), x,C,2, (,x,0,x,), x,C,3,C,404,=,x,0,x
citramal root diacid C,1,(=,x,0,x,),x,C,2,(,x,0,x,)(,x,C,x,),x,C,3,C,404,=,x,0,x
pyrotartr|pyrotartar root diacid
C, 1, (=, x, 0, x,), x, C, 2, (, x, C, x,), x, C, 3, C, 404, =, x, 0, x
itacon root diacid C,1, (=,x,0,x,), x,C,2, (=,x,C,x,), x,C,3,C,404,=,x,0,x
tartar|tartr|dtartar|dtartr|uv|mesotartar|mesotartr pseudosugar unknown x,x
tartar | tartr | uv root diacid
C,1,(=0),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,C,2,Ring,Ring1,
Ring, Ring2, C, 3, Ring, Ring3, C, 4@4, =, x, 0, x
dtartar dtartr root diacid
C,1,(=0),x,Ring,Ring1,.,x,O,o,Ring,Ring2,.,x,O,o',Ring,Ring3,.,x,[C@H],2,Ring,Ri
ng1, Ring, Ring2, [C@H], 3, Ring, Ring3, C, 4@4, =, x, O, x
ltartar | ltartr root diacid
C,1,(=0),x,Ring,Ring1,.,x,0,o,Ring,Ring2,.,x,0,o',Ring,Ring3,.,x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@@H],3,Ring,Ring3,C,4@4,=,x,O,x
mesotartar | mesotartr root diacid
C,1,(=0),x,Ring,Ring1,.,x,0,o,Ring,Ring2,.,x,0,o',Ring,Ring3,.,x,[C@@H],2,Ring,R
ing1,Ring,Ring2,[C@H],3,Ring,Ring3,C,4@4,=,x,O,x
him root diacid
C,x,(=,x,0,x,),x,C,2,Ring,Ring1,C,3,(,x,C,4,Ring,Ring2,C,5,=,x,C,6,C,1,(,x,C,7,R))
ing, Ring2, ), x, Ring, Ring1, ), x, C, 40x, =, x, 0, x
glutaro glutar root diacid
C, 1, (=, x, 0, x,), x, C, 2|a|alpha, C, 3|b|beta, C, 4|g|gamma, C, 4@5, =, x, 0, x
```

```
adipo adip root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,4@6,=,x,0,x
glutacon|glutacono root diacid C,1,(=,x,0,x,),x,C,2,=,x,C,3,C,4,C,4@5,=,x,0,x
mucon | mucono root diacid C,1, (=,x,0,x,), x,C,2,=,x,C,3,C,4,=,x,C,5,C,406,=,x,0,x)
dihydromucon dihydromucono root diacid
C,1,(=,x,0,x,),x,C,2,=,x,C,3,C,4,C,5,C,4@6,=,x,0,x
pimelo|pimel|piler root diacid
C,1,(=,x,0,x,),x,C,2,C,3,C,4,C,5,C,6,C,407,=,x,0,x
subero suber root diacid
x,0,x
azela|azele|azel|lepargyl root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,4@
9, = x, 0, x
sebaco sebac root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C,4010,=,x,0,x
traumat | traumato root diacid
C,1,(=,x,0,x,),x,C,2,=,x,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,4@12,=,x,0,x)
brassylo|brassyl root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C, 10, C, 11, C, 12, C, 4013, =, x, 0, x
thapso thaps root diacid
C,1,(=,x,0,x,),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,
C, 10, C, 11, C, 12, C, 13, C, 14, C, 15, C, 4@16, =, x, 0, x
floion phloion root diacid
C,1,(=,x,0,x,),x,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,(0),x,C,10,(0),x,C,11,C,12,C,13
,C,14,C,15,C,16,C,17,C,4@18,=,x,O,x
folin root diacid
) = 0), x
spiculspor root diacid
C,x,(=,x,0,x,),x,Ring,Ring1,.,x,C,1,(,x,=,x,0,x,),x,(,x,0,x,Ring,Ring2,),x,C,2,C
 ,3,C,4,Ring,Ring2,Ring,Ring1,C,5,(,x,C,4@x,=,x,0,x,),x,C,6,C,7,C,8,C,9,C,10,C,11
 ,C,12,C,13,C,14,C,15
chaulmoogr root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1|
0,C,11,C,12,C,13,[C@@H],x,Ring,Ring1,c,x,c,x,C,x,C,x,Ring,Ring1
pyrocarbon root diacid C, x, (=,x,0,x,), x,0,x,C,40x,=,x,0,x
imidodicarbon iminodicarbon root diacid C, x, (=,x,0,x,), x,N,n,C,40x,=,x,0,x
pyrocarbon root diacid C, x, (=,x,0,x,), x,0,x,C,40x,=,x,0,x
thiodicarbon root diacid C,x,(=,x,0,x,),x,S,x,C,4@x,=,x,0,x
peroxydicarbon root diacid C,x,(=,x,0,x,),x,00,x,C,40x,=,x,0,x
 thioperoxydicarbon root diacid C,x,(=,x,0,x,),x,SS,x,C,4@x,=,x,0,x
chelidon chelid root diacid C,x, (=,x,0,x,),x,clcc(=0)cc(o1),x,C,4@x,=,x,0,x
pamo embon root diacid
C, x, (=, x, 0, x,), x, C1 = CC3 = C(C = CC = C3) C(CC2 = C(C = CC = C4) C4 = CC(, x, C, 4@x, =, x, 0, x,) = C20) = C(x, x, C, x, 
C10,x
 citr root polyacid C,1,C,2,C,3,(,x,0,x,),x,(,x,C,x,),x,C,x,C,x
 isocitr root polyacid C,x,C,x,(,x,0,x,),x,C,x,(,x,C,x,),x,C,x,C,x
 tricarballyl root polyacid C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x
 aconit root polyacid C, x, C, x, = x, C, x, (x, C, x, x, C, x, C
 trimellit root polyacid
 C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
 hemimellit root polyacid
 C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1
```

l,f

Ü

...**.**

1

88

111

n dia

: de

ij

```
hemimellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,(,x,C,x,),x,c,4,c,5,c,6,Ring,Ring1
pyromellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,
Ring1
pyromellitene root root
C,x,c,1,Ring,Ring1,c,2,(,x,C,x,),x,c,3,c,4,(,x,C,x,),x,c,5,(,x,C,x,),x,c,6,Ring,
mellit root polyacid
C, x, c, 1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, (C), x, c, 6, (C), x, Ring, Ring1
trimes root polyacid
C, x, c, 1, Ring, Ring1, c, 2, c, 3, (, x, C, x, ), x, c, 4, c, 5, (, x, C, x, ), x, c, 6, Ring, Ring1
mellophan root polyacid
C, x, c, 1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, c, 6, Ring, Ring1
prehnit root polyacid
C,x,c,1,Ring,Ring1,c,2,(C),x,c,3,(C),x,c,4,c,5,(C),x,c,6,Ring,Ring1
berberon beron root polyacid
C,x,c,2,Ring,Ring1,c,3,(,x,C,x,),x,c,4,c,5,(,x,C,x,),x,c,6,n,1,Ring,Ring1
phthalide root root
0,x,=,x,C,1,Ring,Ring1,0,2,C,3|a|alpha,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring
,Ring1,Ring,Ring2
phthalane|phthalan root root
C,1,Ring,Ring1,0,2,C,3,C,3a,Ring,Ring2,=,x,C,4,C,5,=,x,C,6,C,7,=,x,C,7a,Ring,Rin
q1, Ring, Ring2
phthalo|phthal|orthophthal root diacid
homophthalo homophthal root diacid
C, x, (=, x, 0, x,), x, c, 1, Ring, Ring1, c, 2, (, x, C, x, C, 4ex, =, x, 0, x,), x, c, 3, c, 4, c, 5, c, 6, Ri
ng, Ringl
isophthalo|mphthalo|isophthal|mphthal root diacid
terephthalo|pphthalo|terephthal|pphthal root diacid
C,x,(=,x,0,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,C,4@x,=,x,0,x,),x,c,5,c,6,Ring,R
ing1
uvit root diacid
C,x,(=,x,0,x,),x,c,1,Ring,Ring1,c,2,c,3,(,x,C,4@x,=,x,0,x,),x,c,4,c,5,(C),x,c,6,
Ring, Ring1
leucate leucicacid root root
C,1,(=,x,0,x,),x,(,x,0,10x,),x,C,2,(,x,0,x,),x,C,3,C,4,(,x,C,5,),x,C,x
phenylephrine | phenylephrin root root Oc1cccc(C(O)CNC)c1,x
norepinephrine | norepinephrin | noradrenaline | noradrenalin | arterenol root root
Oc1cc(C(O)CN)ccc10,x
epinephrine|epinephrin|adrenaline|adrenalin root root Oc1cc(C(O)CNC)ccc10,x
adrenalone root root O=C(CNC)c1ccc(O)c(O)c1,x
norephedrine norephedrin root root
OC(C(,x,N,n,)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
ephedrine ephedrin pseudoephedrine pseudoephedrin root root
OC(C(,x,N,n,C)C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1)
taurine | taurin root root 0,10x,S,x, (=0) (=0),x,C,1,C,2,N,n
hypotaurine hypotaurin root root 0,1@x,S,x,(=0),x,C,1,C,2,N,n
cadaverine cadaverin root root N,n,C,1,C,2,C,3,C,4,C,5,N,n'
putrescine putrescin root root N,n,C,1,C,2,C,3,C,4,N,n'
albizzi aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,NC(=0)N,x
```

1

[]

.. **4**

נו

:: :3

ı di

......

```
alan aminoacid ine
C,1,Ring,Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta
homoalan aminoacid ine
\texttt{C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|d|delta|w|}
omega
alanos aminoacid ine
C,1,Ring,Ring1,...x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,N,x,(,x,0,x,)
, x, N, x, =, x, 0, x
alloisoleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@@H],3|b|beta,(,x,
C,4|g|gamma,C,5|d|delta,),x,C,3',
allothreono allothreon aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C)
,4 | g | gamma, ), x, 0, x
allys aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,=0,x
argin aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,nd|ndelta,C,x,(=,x,N,nw'|nomega',),x,N,nw|nomega|ngamma
asparag aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(
aspart aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3,C,4|g|gamma|b|beta,(
=,x,0,x,),x,0,x
azaser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,0,x,C(=0)C=[N]
+] = [N-], X
betaalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nbeta|n3,C,2|a|alpha,C,3|b|beta,Ring,Ring1
buthion aminoacid ine
C,1,Ring,Ring1,...,X,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,CCCC,x
canavan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,0
NC (=N)N, x
carbocyste aminoacid ine
C,1,Ring,Ring1,...x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,CC(=0),x,
0,1@x
citrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
, 5 | d | delta, N, x, C, x, (=, x, 0, x,), x, N, x
cycloleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,Ring,Ring2,C,3|b|beta,C,
4 | g | gamma, C, 5 | d | delta, C, 6, Ring, Ring2
cyste regineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s
cyste aminoacid ine
C,1,Ring,Ring1,...x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,S,s,(=0)(=0),
x,0,10x,
ethion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,C,x,C,x
isoglutam reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,Ring,Ring2,.,x,C,2|a|alpha,Ring,Ring1,C,3|b|bet
a,C,4|g|gamma,Ring,Ring2,C,5|d|delta,(=,x,0,x,),x,N,x
```

```
glutam regineaminoacid ine
\texttt{C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C}
,5|d|delta,(=,x,0,x,),x,N,nd|ndelta|n5
glutam aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
, 5 | d | delta, (=, x, 0, x, ), x, 0, 10x
glyc aminoacid ine C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1
histid aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,4,Ring,Ring2,c,
5,n,1|nt|ntau|im|nim|n'|tau|prefhydro,c,2,n,3|np|npi,Ring,Ring2
homoargin aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,nd|ndelta,C,x,(=,x,N,nw'|nomega',),x,N,nw|nomega
homocitrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,x,C,x,(=,x,0,x,),x,N,x
homocyste reqineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
homocyste aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,s,(=0)(=0),x,0,10x
homoglutam regineaminoacid ine
\texttt{C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C}
 ,5|d|delta,C,6|e|epsilon,(=,x,0,x,),x,N,ne|nepsilon|n6
homophenylalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,c,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,b|beta,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,x,Ring,Ring1,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gamma,C,g|gam
q,Ring2,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring2
homoprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,C,6,Rin
g,Ring2
homoser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,O
homotryptoph aminoacid ane
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,g|gamma,C,3,Rin
g,Ring2,=,x,C,2,N,1,C,7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,
Ring, Ring3
iboten aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C2=CC(=0)NO2,x
 isoleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,[C@H],2|a|alpha,Ring,Ring1,[C@H],3|b|beta,(,x,C)
 ,4|g|gamma,C,5|d|delta,),x,C,3',
 isoser aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,Ring,Ring2,.,x,C,2|a|alpha,Ring,Ring1,(0),x,C,3
 |b|beta,Ring,Ring2
 isoval aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,(,x,C,2',),x,Ring,Ring1,C,3|b|beta,
C,4 | q | qamma
kynuren aminoacid ine
 C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C(=0),x,c,1,Ring,
 Ring2,c,2,(N),x,c,3,c,4,c,5,c,6,Ring,Ring2
 leuc aminoacid ine
 C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,(
 ,x,C,5|d|delta,),x,C,5'
```

: 3

l, f

7

1

: di

1

in.

يقير ...

:: de

```
lys aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon,N,n6|nw|nomega|nepsilon|ne|nz|n'
methion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,S
,x,C,x
mimos aminoacid ine
C,1,Ring,Ring1,...x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,N2C=C(0)C(=0)
C=C2, x
norleuc aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,C,6|e|epsilon
norval aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta
ornith aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
,5|d|delta,N,n5|ndelta|nd
penicillam aminoacid ine
C,1,Ring,Ring1,...,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(C)(C)S,x
phenylalan | 3phenylalan | betaphenylalan aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,x,Ring,Ring2,c,
2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring2
prol aminoacid ine
C,x,Ring,Ring1,...,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,Ring,Ri
3hydroxyprol|hydroxyprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,(0),x,C,4,C,5,R
ing, Ring2
4hydroxyprol aminoacid ine
C,x,Ring,Ring1,.,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,(0),x,C,5,R
ing, Ring2
5hydroxyprol aminoacid ine
ing,Ring2
pyroglutam aminoacid ine
C,x,Ring,Ring1,...,x,N,1|n|nalpha|n2,Ring,Ring2,C,2,Ring,Ring1,C,3,C,4,C,5,(=0),x,
Ring, Ring2
sarcos aminoacid ine
C, 1, Ring, Ring1, ..., x, N, n | nalpha | n2, (,x,C,2 | a | alpha, Ring, Ring1,), x, C, x
selenocyste regineaminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,[Se],se
selenomethion aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,[
Se],x,C,x
ser aminoacid ine
C,1,Ring,Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,0,x
tleuc|tertleuc aminoacid ine
C,1,Ring,Ring1,...x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(,x,C,3',)(,x)
,C,3'',),x,C,3'''
theano thean aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
, x, (=0), x, N, x, C, x, C, x
thiocitrull aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma,C
```

, 5 | d | delta, N, x, C, x, (=, x, S, x,), x, N, x

```
threono|threon aminoacid ine
C, 4 | g | gamma, ), x, 0, x
tryptoph aminoacid ane
C, x, Ring, Ring1, ..., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, C, 3, Ring, Ring2, =,
x,C,2,N,1,C,7a,Ring,Ring3,=,x,C,7,C,6,=,x,C,5,C,4,=,x,C,3a,Ring,Ring2,Ring,Ring3
thyron aminoacid ine
C.x.Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x.C.2 ortho, C.3 m meta, =, x.C.4, (, x.O.x.C.1', Ring, Ring3, =, x.C.2', C.3', =, x.C.4', (,
x,0,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C,5,=,x,C,6,Ring,Ring2
thyrox aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2 ortho,C,3 m meta,(I),x,=,x,C,4,(,x,0,x,C,1',Ring,Ring3,=,x,C,2',C,3',(I),x
x_{1} = x_{1} + x_{2} + x_{3} + x_{4} + x_{5} + x_{5
Ring2
tyros|ptyros|paratyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2 ortho, C,3 m meta, =, x,C,4, (,x,0,x,), x,C,5, =, x,C,6, Ring, Ring2
mtyros | metatyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2 ortho, C,3 m meta, (,x,0,x,),x,=,x,C,4,C,5,=,x,C,6,Ring,Ring2)
orthotyros aminoacid ine
C,x,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,C,1,Ring,Ring2,=,
x,C,2 ortho, (,x,0,x,),x,C,3 m meta, =, x,C,4,C,5,=,x,C,6, Ring, Ring2
val aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,(,x,C,4|g|gam,a)
ma,),x,C,4'|5
willardi aminoacid ine
C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,n2ccc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)nc(=0)
0)2,x
djenkol aminodiacid ine
S,x,C,x,S,x,C,3' | b' | beta',C,2' | a' | alpha',(,x,N,n' | na' | nalpha',),x,C,4@x,=,x,0,x
cyst aminodiacid ine
\texttt{C,1,(=,x,0,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,}
S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,O,x
cvstathion aminodiacid ine
C,1,(=,x,0,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,
0,x
homocyst aminodiacid ine
C,1,(=,x,0,x,),x,Ring,Ring1,..,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
C,4|q|qamma,S,x,S,x,C,4'|g'|gamma',C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nal
pha',),x,C,40x,=,x,0,x
 lanthion aminodiacid ine
 C,1,(=,x,0,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 S,x,C,3'|b'|beta',C,2'|a'|alpha',(,x,N,n'|na'|nalpha',),x,C,4@x,=,x,0,x
 selenocyst aminodiacid ine
 C,1,(=,x,0,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring1,Ring1,C,3|b|beta,
 [Se], x, [Se], x, C, 3' | b' | beta', C, 2' | a' | alpha', (,x,N,n' | na' | nalpha',), x, C, 4@x, =, x, 0,
 selenocystathion aminodiacid ine
 C,1,(=,x,0,x,),x,Ring,Ring1,.,x,N,n|nalpha|n2,C,2|a|alpha,Ring,Ring1,C,3|b|beta,
 C, 4 | g | gamma, [Se], x, C, 3' | b' | beta', C, 2' | a' | alpha', (, x, N, n' | na' | nalpha', ), x, C, 40x, = 0
  , x, 0, x
 in | ine enderaminoacid ine 0,80x,.,x,0,50x
 an ane enderaminoacid ane 0,80x,.,x,0,50x
```

```
yl enderaminoacid yl 0,80x
ol enderaminoacid suffix 0,80x
aceglutamide | aceglutamid root root O=C(,x,0,1@x,)C(NC(C)=0)CCC(N)=0,x
methionol root root CSCCCO, x
tryptophol root root
OCC, x, c, 3, Ring, Ring1, c, 2, n, 1, c, 7a, Ring, Ring2, c, 7, Ring, Ring1, c, 6, c, 5, c, 4, c, 3a, Rin
g,Ring2
cysteamine|cysteamin root root N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,s
histamine|histamin root root
N, n | nalpha | n2 | nomega, C, a | alpha, C, b | beta, C, 4, Ring, Ring2, =, x, C, 5, N, 1 | nt | ntau, C, 2, =
 ,x,N,3|np|npi,Ring,Ring2
methioninamine methioninamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,x
 tryptamine tryptamin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
q3, =, x, C, 7, C, 6, =, x, C, 5, C, 4, =, x, C, 3a, Ring, Ring2, Ring, Ring3
melatonin root root
N,n|nalpha|n2|nomega,(C(=0)C),x,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,a|alpha|n2|nomega,(C(=0)C),x,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,b|beta,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|alpha,C,a|a
7a, Ring, Ring3, =, x, C, 7, C, 6, =, x, C, 5, (OC), x, C, 4, =, x, C, 3a, Ring, Ring2, Ring, Ring3
 serotonin root root
N,n|nalpha|n2|nomega,C,a|alpha,C,b|beta,C,3,Ring,Ring2,=,x,C,2,N,1,C,7a,Ring,Rin
q3, =, x, C, 7, C, 6, =, x, C, 5, (0), x, C, 4, =, x, C, 3a, Ring, Rin
 tyramine|tyramin|tyrosamine|tyrosamin root root
N,n \mid nalpha \mid n2 \mid nomega,C,a \mid alpha,C,b \mid beta,C,1,Ring,Ring2,=,x,C,2 \mid ortho,C,3 \mid m \mid meta,
 =, x, C, 4, (, x, 0, x, ), x, C, 5, =, x, C, 6, Ring, Ring2
 cystamine cystamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,S,x,C,3'|b'|beta',C,2'|a'|alpha'
 ,N,n'|na'|nalpha'
 selenocystamine|selenocystamin root root
alpha', N, n' | na' | nalpha'
 cystathionamine cystathionamin root root
N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,C,3'|b'|beta',C,2'|a
 '|alpha', N, n'|na'|nalpha'
 homocystamine homocystamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,S,x,S,x,C,4'|g'|gamma',C
  ,3'|b'|beta',C,2'|a'|alpha',N,n'|na'|nalpha'
 lanthionamine lanthionamin root root
 N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha,C,3|b|beta,S,x,C,3'|b'|beta',C,2'|a'|alpha',N,n|nalpha|n2|nomega,C,2|a|alpha',N,n|nalpha|n2|nomega,C,2'|a'|alpha',N,n|nalpha|n2|nomega,C,2'|a'|alpha',N,n|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalpha|nalph
  '|na'|nalpha'
 methional root root 0,x,=,x,C,1,C,2,C,3,S,x,C,x
 glycero sugar hexose 0, x, =, x, C, 1, [C@H](, 2, 0, x,), x, C, 3, 0, x
 erythro erythr sugar hexose
 0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@H](,3,0,x,),x,C,4,0,x
 threo|thre sugar hexose 0, x, =, x, C, 1, [C@@H](,2,0,x,), x, [C@H](,3,0,x,), x, C, 4, 0, x
 ribo|rib sugar hexose
 0, x, =, x, C, 1, [C@H](, 2, 0, x,), x, [C@H](, 3, 0, x,), x, [C@H](, 4, 0, x,), x, C, 5, 0, x
 arabino arabin arab sugar hexose
 0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@H](,3,0,x,),x,[C@H](,4,0,x,),x,C,5,0,x
 xylo|xyl sugar hexose
 0, x, =, x, C, 1, [C@H](, 2, 0, x,), x, [C@GH](, 3, 0, x,), x, [C@H](, 4, 0, x,), x, C, 5, 0, x
 lyxo lyx sugar hexose
 0, x, =, x, C, 1, [C@@H](, 2, 0, x,), x, [C@@H](, 3, 0, x,), x, [C@H](, 4, 0, x,), x, C, 5, 0, x
```

```
Last Last Last Control Control
```

```
allo sugar hexose
0, x, = x, C, 1, [C@H] (, 2, 0, x,), x, [C@H] (, 3, 0, x,), x, [C@H] (, 4, 0, x,) [C@H] (, 5, 0, x,), x, C, 6
altro altr sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@H](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C,
6,0,x
gluco|gluc sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@GH](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C,
6,0,x
manno mann sugar hexose
0, x, =, x, C, 1, [C@@H](, 2, 0, x,), x, [C@@H](, 3, 0, x,), x, [C@H](, 4, 0, x,) [C@H](, 5, 0, x,), x, C
, 6, 0, x
gulo gul sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@H](,3,0,x,),x,[C@@H](,4,0,x,)[C@H](,5,0,x,),x,C,
ido sugar hexose
0,x,=,x,C,1,[C@@H](,2,0,x,),x,[C@H](,3,0,x,),x,[C@@H](,4,0,x,)[C@H](,5,0,x,),x,C
,6,0,x
galacto|galact|dulc sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@@H](,3,0,x,),x,[C@@H](,4,0,x,)[C@H](,5,0,x,),x,C
talo tal sugar hexose
0, x, =, x, C, 1, [C@@H](, 2, 0, x,), x, [C@@H](, 3, 0, x,), x, [C@@H](, 4, 0, x,) [C@H](, 5, 0, x,), x,
C, 6, 0, x
boivin sugar hexose
0,x,=,x,C,1,[C@H],2,[C@H],3,0,x,),x,[C@GH],4,0,x,)[CGH],5,0,x,),x,C,6
digitox sugar hexose
0, x, =, x, C, 1, C, 2, [C@H](,3,0,x,), x, [C@H](,4,0,x,)[C@H](,5,0,x,), x, C, 6
oli sugar hexose
0, x, =, x, C, 1, [C@H], 2, [C@GH], 3, 0, x, x, x, [C@GH], 4, 0, x, [C@GH], 5, 0, x, x, x, C, 6
oliv sugar hexose
0,x,=,x,C,1,[C@H],2,[C@GH](,3,0,x,),x,[CGH](,4,0,x,)[CGH](,5,0,x,),x,C,6
glucohept sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@H](,3,0,x,),x,[C@H](,4,0,x,),x,[C@GH](,5,0,x,)[CGGG]
@H](,6,0,x,),x,C,7,0,x
fuco fuc sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@GH](,3,0,x,),x,[C@GH](,4,0,x,)[CGH](,5,0,x,),x,C
quinovo quinov sugar hexose
0,x,=,x,C,1,[C@H](,2,0,x,),x,[C@GH](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C,
rhamno rhamn sugar hexose
0,x,=,x,C,1,[C@@H](,2,0,x,),x,[C@@H](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C
, 6
rhodeo rhode sugar hexose
O, X, =, X, C, 1, [C@H](,2,0,X,), X, [C@@H](,3,0,X,), X, [C@@H](,4,0,X,) [C@H](,5,0,X,), X, C
thymino thymin sugar hexose
O, x, =, x, C, 1, [C@H], 2, [C@H](,3,0,x,), x, [C@H](,4,0,x,), x, C, 5, 0, x
qalactosamine|qalactosamin|chondrosamine|chondrosamin sugar trivial
O, x, =, x, C, 1, [C@H](, 2, N, x,), x, [C@@H](, 3, 0, x,), x, [C@@H](, 4, 0, x,) [C@H](, 5, 0, x,), x, C
,6,0,x
glucosamine glucosamin sugar trivial
6,0,x
```

```
mannosamine mannosamin sugar trivial
0,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C
,6,0,x
fucosamine fucosamin sugar trivial
O, x, =, x, C, 1, [C@H](, 2, N, x,), x, [C@@H](, 3, 0, x,), x, [C@@H](, 4, 0, x,) [C@H](, 5, 0, x,), x, C
quinovosamine quinovosamin sugar trivial
O, x, =, x, C, 1, [C@H](, 2, N, x,), x, [C@@H](, 3, 0, x,), x, [C@H](, 4, 0, x,) [C@H](, 5, 0, x,), x, C,
rhamnosamine rhamnosamin sugar trivial
O, x, =, x, C, 1, [C@@H](, 2, N, x,), x, [C@@H](, 3, O, x,), x, [C@H](, 4, O, x,) [C@H](, 5, O, x,), x, C
, 6
glucal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x
rhamnal sugar trivial
C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6
galactal sugar trivial
C, 1, Ring, Ring1, =, x, C, 2, [C@@H], 3, (0), x, [C@@H], 4, (0), x, [C@H], 5, (01), x, C, 6, 0, x
glucamine sugar trivial
N,n,C,1,[C@H](,2,0,x,),x,[C@@H](,3,0,x,),x,[C@H](,4,0,x,)[C@H](,5,0,x,),x,C,6,0,
sucr sugar disugar
OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)
)02,x
trehal sugar disugar
O[C@H]1[C@H](O)[C@@H](CO)O[C@H](O[C@H]2[C@@H](O)[C@H](O)[C@H](O)[C@H](CO)O2)[C@
@H]10,x
melezit sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O[C@@]2(CO)[C@@H](O[C@H]3O[C@H](CO)[C@
@H](O)[C@H](O)[C@H]3O)[C@H](O)[C@@H](CO)O2)O1,x
stachy|lupe sugar disugar
O[C@H]1[C@@H](CO)O[C@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O[C@]4(CO)O[C@H](CO)[C@@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[C@H](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO)[CO](CO](CO](CO)[CO]
O) [C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)[C@H](O)[C@H](O)[C@H]2O)[C@H](O)[C@H]1O,
lact sugar disugar
OC[C@H]10[C@@H](O[C@@H]([C@H](O)[C@@H](O)[C@@H](O)02)[C@H]2CO)[C@H](O)[C@@H](O)[
C@H|10,x
malt maltobi sugar disugar
O[C@@H]1[C@@H](O)[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)O[C@H](CO)[C
@H]10,x
maltotri sugar disugar
O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]10[C@@H]2[C@@H](CO)O[C@H](O[C@@H]3[C@@
H](CO)OC(O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O,x
maltotetra sugar disugar
O[C@@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O)O[C@@H]4CO)O)O[C@@H]1CO)[C@@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](O)[CW](
 @@H]10[C@@H]2[C@H](O)[C@H]([C@H](O[C@H](O)[C@H]30)[C@H](O)[C@H]30)[C@H]30)
 (CO)(O2)(O, X)
 maltopenta sugar disugar
 O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1[C@@H](CO)O[C@H](O[C@H]3[C@H](O)[
 \texttt{C@H}] \ ( \texttt{[C@@H]} \ ( \texttt{O[C@H]} 4 \texttt{[C@H]} \ ( \texttt{O)} \texttt{[C@H]} \ ( \texttt{C@@H]} 5 \texttt{[C@H]} \ ( \texttt{O)} \texttt{[C@H]} \ ( \texttt{C@@H]} 5 \texttt{CO} ) \\
 )0)0[C@@H]4C0)0)0[C@@H]3C0)0)[C@H](0)[C@H]10,x
 maltohexa sugar disugar
 O[C@@H]([C@@H](O[C@H]3[C@H](O)[C@H]([C@@H](O[C@H]6[C@H](O)[C@H]([C@@H](O)O[C@@H]
 ]4[C@H](O)[C@H]([C@H](O[C@H](O)[C@H]50)[C@H](O)[C@H]50)[C@H](O)04)0)[
 C@@H](CO)O2)O,x
```

```
melibi sugar disugar
O(C@H)1(C@GH)(OC(C@H)(CGGH)(O)(CGH)(O)(CGH)2O)O(CGH)2O)O(CGH)(CO)(CGH)(O)(CGGH)
cellobi sugar disugar
OC[C@@H]1[C@@H](O)[C@H](O)[C@H](O)[C@H](O[C@@H]2[C@@H](CO)O[C@@H](O)[C@H](O)[C@
H]20)01,x
cellotri sugar disugar
O[C@H]([C@H]10)[C@H](O[C@H]2[C@H](0)[C@H]([C@H](0]C@H]3[C@H](0)[C@H](C(0)0[C@@H]
3CO)O)O[C@@H]2CO)O)O[C@H](CO)[C@H]10,x
cellotetra sugar disugar
OC(O[C@@H](CO)[C@@H]10[C@H]2[C@@H](O)[C@H](O)[C@@H](O[C@@H]3[C@@H](O)[C@H](O)[C@
@H](O[C@@H]4[C@@H](O)[C@H](O)[C@H](O)[C@H](CO)O4)[C@H](CO)O3)[C@H](CO)O2)[C@@H]
 (O) [C@@H] 10, x
cellopenta sugar disugar
OC(O[C@H]1CO)[C@@H](O)[C@@H]([C@H]1O[C@H]2[C@@H](O)[C@H](O)[C@H](O[C@H](O[C@H]
  (CO) \ [C@@H] \ 30 \ [C@@H] \ 4 \ [C@@H] \ (O) \ [C@H] \ (O) \ [C@H] \ (O) \ [C@@H] \ (O) \ [C@@H] \ (O) \ [C@@H] \ (O) \ [C@H] \ (O) \ [C@
H](CO)O5)[C@H](CO)O4)[C@@H](O)[C@@H]3O)[C@H](CO)O2)O,x
 chitobi sugar disugar
N,n,[C@@H]([C@H](0)O[C@@H]2CO)[C@@H](0)[C@@H]2O[C@H](01)[C@H](,x,N,n',)[C@@H](0)
 [C@H](O)[C@H]1CO,x
 chitotri sugar disugar
N,n,[C@@H](C(0)O[C@@H]3CO)[C@@H](0)[C@@H]3O[C@H](0[C@@H]1CO)[C@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[(,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@M](,x,N,n',)[C@@H](,x,N,n',)[C@@H](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n',)[C@M](,x,N,n'
 raffin melit melitri sugar disugar
OC[C@H]10C(OC[C@H]20C(O[C@@]3(CO)[C@@H](O)[C@H](O)[C@@H](CO)O3)[C@H](O)[C@@H](O)
 [C@@H] 20) [C@H] (0) [C@@H] (0) [C@H] 10, x
 gentiobi sugar disugar
O[C@H]1[C@H](OC[C@H]([C@@H](O)[C@H](O)[C@H]2O)O[C@H]2O)O[C@H](CO)[C@@H](O)[C@@H]
 10,x
 palatin sugar disugar
 OC[C@@]1(O)O[C@H](CO[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2)[C@@H](O)[C@@H]
 10,x
 turan sugar disugar
 O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@GH]1C(O)(CO)OC[C@GH](O)[CGH]1O, x
 ose endersugar ose x,x
 itol endersugar itol x,x
 ityl endersugar makefree x,x
 ide | id | oside | osid endersugar oside x,x
 on ono endersugar on x,x
 uron urono endersugar uron x,x
 ar aro endersugar ar x,x
 odialdo odiald endersugar dialdo x,x
 oxirose oxiros pyranose unknown 2,x
 oxetose oxetos pyranose unknown 3,x
 furanose|furanos|ofuranose|ofuranos pyranose unknown 4,x
 pyranose|pyranos|opyranose|opyranos pyranose unknown 5,x
 septanose | septanos | oseptanose | oseptanos | pyranose | unknown 6, x
 tetro multsugar unknown 4,x
 pento multsugar unknown 5,x
 hexo multsugar unknown 6,x
 hepto multsugar unknown 7,x
 octo multsugar unknown 8,x
 nono multsugar unknown 9,x
 deco multsugar unknown 10,x
 ulo|ul structsugarender ulose C=0,x
  osamine structsugarender osamine N,x
  deoxy deoxy unknown C,x
```

```
inositol pseudosugar unknown x,x
inositol root root OC1C(O)C(O)C(O)C(O)C1O,x
mesoinositol myoinositol root root
O,x,[C@H],1,Ring,Ring1,[C@@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),
x, [C@@H], 6, Ring, Ring1, 0, x
scylloinositol root root
O,x,[C@H],1,Ring,Ring1,[C@H],2,(O),x,[C@eH],3,(O),x,[C@H],4,(O),x,[C@eH],5,(O),x
,[C@@H],6,Ring,Ring1,0,x
epiinositol root root
O,x,[C@H],1,Ring,Ring1,[C@@H],2,(O),x,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@@H],5,(O)
,x,[C@@H],6,Ring,Ring1,0,x
dinositol root root O[C@H]1[C@@H](O)[C@H](O)[C@H](O)[C@@H](O)[C@@H]10,x
linositol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](O)[C@H](O)[C@H]10,x
quebrachitol root root O[C@@H]1[C@H](O)[C@@H](O)[C@H](O)[C@H]10,x
muram pseudosugar unknown x,x
muram root root
CC(C)O,x,[C@H],3,Ring,Ring1,[C@H],4,(O),x,[C@@H],5,(,x,C,6,O,x,),x,O,x,[C@H],1,(
O), x, [C@H], 2, (,x,N,n,), x, Ring, Ring1
neuramin pseudosugar unknown x,x
neuramin root root
C,x,[C@@],2,Ring,Ring1,(0),x,0,x,[C@@H],6,(,x,[C@H],7,(0),x,[C@H],8,(0),x,C,9,0,
x, ), x, [C@H], 5, (,x,N,n,), x, [C@@H], 4, (0), x,C,3,Ring,Ring1
sial pseudosugar unknown x,x
sial root root
C.x.[C@@].2.Ring.Ring1,(0),x.0.x.[C@@H].6,(.x.[C@H].7,(0),x.[C@H].8,(0),x.C.9,0.
adenos adenyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
q,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3
,c,4,Ring,Ring3,Ring,Ring2
cytid cytidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,1,Ring,Ring2,c,2,(=0),x,n,3,c,4,(,x,N,n|n4,),x,c,5,c,6,Ring,Ring2
guanos | guanyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(=0),x,N,1,c,2,(,x,N,n|n2,
),x,n,3,c,4,Ring,Ring3,Ring,Ring2
inos nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(0),x,n,1,c,2,n,3,c,4,Ring
,Ring3,Ring,Ring2
thymid thymidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,C,2',[C@@H],1',(O,x,Ring,Ring1,),x
n, 1, Ring, Ring2, c, 2, (=0), x, n, 3 | n, c, 4, (=0), x, c, 5, (C), x, c, 6, Ring, Ring2
urid uridyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,1,Ring,Ring2,c,2,(=0),x,n,3|n,c,4,(=0),x,c,5,c,6,Ring,Ring2
xanthos | xanthoyl | xanthonyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
g,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(0),x,n,1,c,2,(0),x,n,3,c,
4, Ring, Ring3, Ring, Ring2
orotid|orotidyl nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
q,Rinq1,),x,n,1,Rinq,Rinq2,c,2,(=0),x,n,3,c,4,(=0),x,c,5,c,6,(C(=0)0),x,Ring,Rin
g2
```

```
cordycep nucleotide nucleotide
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring
1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,Ring,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3,c,4,R
ing,Ring3,Ring,Ring2
adenyl loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(,x,N,n|n6,),x,n,1,c,2,n,3,c,4,Ring,Ring3,Ring,Ring2
cytidyl loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,
3,c,4,(,x,N,n,),x,c,5,c,6,Ring,Ring2
guanyl loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing,Ring3,c,6,(=0),x,n,1,c,2,(,x,N,n|n2,)n,3,c,4,Ring,Ring3,Ring,Ring2
inos loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,9,Ring,Ring2,c,8,n,7,c,5,R
ing, Ring3, c, 6, (0), x, n, 1, c, 2, n, 3, c, 4, Ring, Ring3, Ring, Ring2
thymidyl loveracid root
P,x, (=0),x, (,x,0,1@o',),x, (,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(0), x, C, 2', [C@@H], 1', (0, x, Ring, Ring1,), x, n, 1, Ring, Ring2, c, 2, (=0), x, n, 3 | n, c, 4, (=0)
), x, c, 5, (C), x, c, 6, Ring, Ring2
uridyl loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Ring,Ring1,),x,n,1,Ring,Ring2,c,2,(=O),x,n,
3 \mid n, c, 4, (=0), x, c, 5, c, 6, Ring, Ring 2
xanthoyl | xanthonyl loveracid root
P,x,(=0),x,(,x,0,1@o',),x,(,x,0,1@o,),x,0,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',
(0), x, [C@@H], 2', (0), x, [C@@H], 1', (0, x, Ring, Ring1,), x, n, 9, Ring, Ring2, c, 8, n, 7, c, 5, R
ing,Ring3,c,6,(0),x,n,1,c,2,(0),x,n,3,c,4,Ring,Ring3,Ring,Ring2
purineriboside root root
O,x,C,5',[C@@H],4',Ring,Ring1,[C@@H],3',(O),x,[C@@H],2',(O),x,[C@@H],1',(O,x,Rin
q,Rinq1,),x,n,9,Rinq,Rinq2,c,8,n,7,c,5,Ring,Ring3,c,6,n,1,c,2,n,3,c,4,Ring,Ring3
,Ring,Ring2
thuj root root
C,3,Ring,Ring1,C,2,C,1,Ring,Ring2,(,x,C,7,(,x,C,8,),x,C,9,),x,C,6,C,5,Ring,Ring2
,C,4,Ring,Ring1,(,x,C,10,),x
car root root
C,1,Ring,Ring1,Ring2,Ring2,C,2,C,3,(,x,C,4,C,5,C,6,Ring,Ring1,(,x,C,7,Ring,Ring2,
(,x,C,8,),x,C,9,),x,),x,C,10
norcar root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,C,5,C,6,Ring,Ring1,(,x,C,7,Ring,Ring2,),x
pin root root
C, 2, Ring, Ring1, (,x,C,10,), x,C,3,C,4,C,5, (,x,C,7,Ring,Ring2,), x,C,6, (,x,C,8,) (,x,C,8,)
C,9,),x,C,1,Ring,Ring2,Ring,Ring1
norpin root root
C,2,Ring,Ring1,C,3,C,4,C,5,(,x,C,7,Ring,Ring2,),x,C,6,C,1,Ring,Ring2,Ring,Ring1
camphor loveracid root
C,10,C,1,Ring,Ring1,Ring2,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,(,x,C,
8,),x,(,x,C,9,),x,Ring,Ring2
camphor root root
C,10,C,1,Ring,Ring1,Ring2,Ring2,C,2,(=0),x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7
(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
```

```
norcamphor root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(=0),x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring
,Ring2
camphorquinone camphoroquinone root root
C, 10, C, 1, Ring, Ring1, Ring2, C, 2, (=0), x, C, 3, (=0), x, C, 4, (, x, C, 5, C, 6, Ring, Ring1, C, 10, C, 10
), x, C, 7, (,x, C, 8, ), x, (,x, C, 9, ), x, Ring, Ring2
borne|born|camphane|camphan|bornylane|bornylan|isoborne|isoborn root root
C, 2, Ring, Ring1, C, 3, C, 4, Ring, Ring2, C, 5, C, 6, C, 1, Ring, Ring1, (,x,C,7, Ring, Ring2, (,x,
C, 8, ), x, C, 9, ), x, C, 10
camphan loveracid root
C,1,Ring,Ring1,Ring,Ring2,O,2,C,3,(=0),x,C,4,(,x,C,5,C,6,Ring,Ring1,),x,(,x,C,7,Ring,Ring1,),x,(,x,C,7,Ring,Ring1,),x,(,x,C,7,Ring,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1,Ring1
 (,x,C,x,)(,x,C,x,),x,Ring,Ring2,),x,C,x
norborne|norborn|norborna root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2
norbornadien|norbornadiene|25norbornadien|25norbornadiene root root
C, 1, Ring, Ring1, Ring2, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, Ring, Ring1,), x, C, 7, Ring
norbornen|norbornene|2norbornen|2norbornene root root
C,1,Ring,Ring1,Ring2,C,2,=,x,C,3,C,4,(,x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ri
nq2
5norbornen|5norbornene root root
C,1,Ring,Ring1,Ring2,C,2,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,C,7,Ring,Ri
camphene camphen root root
x,C,5,C,6,Ring,Ring1,),x,C,7,Ring,Ring2
phosgene phosgen root root ClC(=0)Cl,x
triphosgene | triphosgen root root C(Cl)(Cl)(Cl)OC(=0)OC(Cl)(Cl)(Cl),x
glyoxyl root root C,1,C,2|w| omega, =, x,0,x
pyruv root root C,1,C,2,(=,x,0,x,),x,C,3|w| omega
glycerol|snglycerol|racglycerol pseudosugar unknown x,x
qlycerol|snglycero|racglycerol|racglycero|glycero|glycerine root root
0,101 a alpha, C, x, C, x, (, x, 0, 102 b beta,), x, C, x, 0, 103 g gamma
glycerin root root 0.101|a|alpha,C,x,C,x,(,x,0,102|b|beta,),x,C,x,0,103|g|gamma
glycerone|glyceron root root 0,1@1|a|alpha,C,x,C,x,(=0),x,C,x,0,1@3|g|gamma
in anoin glycerin root
0,101 a alpha, C, x, C, x, (, x, 0, 102 b beta,), x, C, x, 0, 103 g gamma a' alpha'
gerani geran root root
C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,/,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
tetrahydrogerani | geran root root
C,1,C,2,C,3,(,x,C,x,),x,C,4,C,5,C,6,C,7,(,x,C,x,),x,C,8
ner root root
C,1,/,x,C,2,=,x,C,3,(,x,C,x,),x,\\,x,C,4,C,5,C,6,=,x,C,7,(,x,C,x,),x,C,8
phyt root root
C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,C,x,(,x,C,x,),x,
C, x, C, x, C, x, C, x, (, x, C, x,), x, C, x
citral root root
0, x, =, x, C, x, C, x, =, x, C, x, (, x, C, x, ), x, C, x, C, x, C, x, =, x, C, x, (, x, C, x, ), x, C, x
 ethylcitral root root
0, x, =, x, C, x, C, x, =, x, C, x, (, x, C, x, ), x, C, x, C, x, C, x, C, x, C, x, (, x, C, x, ), x, C, x, C, x
 citronell|betacitronell|baran root root CCC(C)CCC=C(C)C,x
 linalo root root C(CCC=C(C)C)(C=C)C,x
 dihydrolinalo root root C(CCC=C(C)C)(CC)C,x
 tetrahydrolinalo root root C(CCCC(C)C)(CC)C,x
 lavandul root root CC(C(=C)C)CC=C(C)C,x
 tetrahydrolavandul root root CC(C(C)C)CCC(C)C,x
```

```
farnes root root
C,1,C,2,=,x,C,3,(C),x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8,C,9,C,10,=,x,C,11,(C)C,x
ocimene root C,1,=,x,C,2,C,3,(C)=,x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8
alloocimene allocimen root root
C, 1, C, 2, (C) = x, C, 3, C, 4, = x, C, 5, (C), x, C, 6, = x, C, 7, C, 8
nerolid root root C(C)(C=C)CCC=C(C)CCC=C(C)C,x
all root root C,1|a|alpha,C,2|b|beta,=,x,C,3|g|gamma
isoall root root C,1|a|alpha,=,x,C,2|b|beta,C,3|g|gamma
homoall root root C,1|a|alpha,C,2|b|beta,C,3|g|gamma,=,x,C,4|d|delta
methall root root C,1,C,2,(,x,C,x,),x,=,x,C,3
triazeno root root N,4@1,=,x,N,2,N,3
vin root root C,1|a|alpha,=,x,C,2|b|beta
hydrazine|hydrazin root root N,1|n,N,2|n'
dithioiminocarbonate root root S,1@s,C,x,(=,x,N,n,),x,S,1@s'
urea | carbamide | carbamid root root N, 1 | n, C, 2, (x, =, x, 0, 0,), x, N, 3 | n'
sulfocarbamide sulfocarbamid sulfourea root root
N, 1 \mid n, C, 2, (x, =, x, S, s,), x, N, 3 \mid n'
biurea root root N,1,C,2,(=0),x,N,3,N,4,C,5,(=0),x,N,6
guanyl root root C,40x,(=N),x,N,x
uronium root root N, 1 | n, C, 2, (x, N, 3 | n', ), x, =, x, [0+], o
ureido root root N,401|n,C,2,(,x,=,x,0,o,),x,N,3|n'
ureylene ureylen root bridge N,401|n,C,2,(,x,=,x,0,o,),x,N,403|n'
carbanilide carbanilid root root
c,6,Ring,Ring1,c,5,c,4,c,3,c,2,c,1,Ring,Ring1,N,n,C,x,(,x,=,x,0,o,),x,N,n',c,1',
Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
tms root root [Si], 40x, (C) (C) (C), x
tbdms root root [Si], 4@x, (C(C)(C)C)(C)(C), x
plumb root root [Pb],1
sil root root [Si],x
stann root root [Sn],x
bor root root [B],x
germ root root [Ge],x
amine amin ammonia root root N,n
phosphine phosphin root root P,x
arsine arsin root root [As],x
hydrogen root root [H],40x
deuterium root root [2H],4@x
tritium root root [3H],4@x
hydrido root root [H-],40x
deuterido root root [2H-],4@x
lithio root root [Li], 40x
sodio root root [Na],40x
potassio kalio root root [K], 40x
fluoro | fluor root root F,40x
chloro chlor root root Cl,40x
chlorosyl root root Cl,4@x,=0,x
chloryl root root Cl,40x, (=0)=0,x
perchloryl root root Cl,4@x,(=0)(=0)=0,x
borono root root [B],40x,(0)0,x
lithium root metal [Li],x
sodium | natrium root metal [Na], x
potassium kalium root metal [K], x
rubidium root metal [Rb],x
cesium root metal [Cs],x
francium root metal [Fr],x
beryllium | glucinium root metal [Be], x
magnesium root metal [Mg],x
```

calcium root metal [Ca], x strontium root metal [Sr], x barium root metal [Ba],x radium root metal [Ra], x scandium root metal [Sc],x yttrium root metal [Y],x lanthanum root metal [La], x cerium root metal [Ce],x praesodymium praseodymium root metal [Pr], x neodymium root metal [Nd], x promethium root metal [Pm], x samarium root metal [Sm],x europium root metal [Eu],x gadolinium root metal [Gd],x terbium root metal [Tb], x dysprosium root metal [Dy],x holmium root metal [Ho], x erbium root metal [Er],x thulium root metal [Tm],x ytterbium root metal [Yb],x lutetium | cassiopeium root metal [Lu], x actinium root metal [Ac],x thorium root metal [Th], x protactinium root metal [Pa], x uranium root metal [U],x neptunium root metal [Np],x plutonium root metal [Pu], x americium root metal [Am], x curium root metal [Cm],x berkelium root metal [Bk],x californium root metal [Cf],x einsteinium root metal [Es], x fermium root metal [Fm],x mendelevium root metal [Md], x nobelium root metal [No], x lawrencium root metal [Lr], x titanium root metal [Ti], x zirconium root metal [Zr], x hafnium root metal [Hf],x vanadium root metal [V],x niobium root metal [Nb],x tantalum root metal [Ta],x chromium root metal [Cr],x molybdenum root metal [Mo],x tungsten root metal [W],x manganese root metal [Mn], x technetium root metal [Tc], x rhenium root metal [Re], x iron root metal [Fe],x ruthenium root metal [Ru], x osmium root metal [Os], x cobalt root metal [Co], x rhodium root metal [Rh], x iridium root metal [Ir],x nickel root metal [Ni], x palladium root metal [Pd],x platinum root metal [Pt],x

silver argent root metal [Ag], x gold root metal [Au],x zinc root metal [Zn],x cadmium root metal [Cd],x mercury root metal [Hg], w boron root nonmetal [B],x aluminum alane root metal [Al], x gallium root metal [Ga], x indium root metal [In],x thallium root metal [T1],x carbon root nonmetal [C], x silicon root nonmetal [Si], x germanium root metal [Ge], x tin root metal [Sn],x lead root metal [Pb],x nitrogen root nonmetal [N],x phosphorus root nonmetal [P], x arsenic root nonmetal [As], x antimony stibium root metal [Sb], x bismuth root metal [Bi], x oxygen root nonmetal [0], x sulfur root nonmetal [S], x selenium root nonmetal [Se], x tellurium root nonmetal [Te], x polonium nonroot metal [Po], x fluorine root nonmetal [F],x chlorine root nonmetal [Cl], x bromine root nonmetal [Br], x iodine root nonmetal [I],x astatine root nonmetal [At],x helium root nonmetal [He], x neon root nonmetal [Ne], x argon root nonmetal [Ar],x krypton root nonmetal [Kr], x xenon root nonmetal [Xe],x radon root nonmetal [Rn], x bromo brom root root Br, 40x iodo | iod root root I,40x iodosyl|iodoso root root I,4@x,=0,x iodyl|iodoxy root root I,4@x,(=0)=0,x deutero deuterio root root [2H],4@x nitro root root [N+], 40x, (=0) [0-], xacinitro root root [N+],8@x,(O)[O-],x nitroso|nitros|nitrosyl root root N=0,40x nitrosamido root root N,40x,N=0,x nitrosamide root root NN=0,x nitrosonium root root [NH0+],x,=0,x isonitroso isonitros root root N,80x,0,x hydroxy hydroxo root root 0,40x hydroxyl root root 0,400 hydroseleno root root [Se],40x hydrotelluro root root [Te],40x cyano|cyanogen root root C#N,4@x isocyano isonitrilo root root [N+]#[C-],4@x cyanato root root OC#N,4@x

copper root metal [Cu], x

```
isocyanato root root N=C=0,40x
thiocyanato root root SC#N,4@x
isothiocyanato root root N=C=S,4@x
selenocyanato root root [Se]C#N,4@x
isoselenocyanato root root N=C=[Se],4@x
diazo root root [N+], 80x, = [N-], x
diazoate | diazoat root root [N+], 8@x, =N, x, [O-], x
azido triazo root root N, 40x, = [N+] = [N-], x
oxo|keto root root 0,80x
oxido root root [O-],40x
thioxo|thiono root root S,8@x
sulfido root root [S-],40x
selenoxo root root [Se],8@x
telluroxo root root [Te],80x
mercapto root root S,40x
hydroperoxy root root 0,40x,0,x
carboxy root root C,40x,(=,x,0,x,),x,0,x
amidino root root C,40x,(,x,N,x,)=,x,N,x
aminoiminometh root root C,x,(=,x,N,x,),x,N,x
sulfo root heterolover S,40x,(=0),x,(=0),x,0,x
sulfoxy root root 0,40x,S,x,(=0),x,(=0),x,0,x
sulfoamido root root N, 40x, S, x, (=0), x, (=0), x, 0, x
sulfino root root S,40x, (=0),x,0,x
sulfeno root root S,4@x,0,x
sulfonato root root S, 40x, (=0), x, (=0), x, [0-], x
phosphonato | phosphato root root P,40x,(=0),x,([0-]),x,[0-],x
hydrogenphosphato root root P, 40x, (=0), x, (0), x, [0-], x
dihydrogenphosphato root root P,4@x,(=0),x,(0),x,0,x
phosphinato root root P,4@x,(=0),x,[0-],x
phosphono phosphoro infix infix P,40x, (=0),x,(,x,0,100',),x,0,100
phospho root heterolover P,4@x,(=0),x,(0),1@x,0,1@x
diphospho root heterolover P,40x, (=0),x,(0),10x,0,x,P,x,(=0),x,(0),10x,0,10x
triphospho root heterolover
P,40x, (=0), x, (0), 10x, 0, x, P, x, (=0), x, (0), 10x, 0, x, P, x, (=0), x, (0), 10x, 0, 10x
phosphinico root root P,80x,(=0),x,0,100
arsonato root root [As], 40x, (=0), x, ([O-]), x, [O-], x
arsinato root root [As], 40x, (=0), x, [0-], x
arsono arsoro root root [As], 40x, (=0), x, (,x,0,100',),x,0,100
arsinico root root [As],8@x,(=0),x,0,1@o
mesyl root root S,40x,(=0),x,(=0),x,C,x
-part2-toluene root root C,4@a|alpha
-part2-cumene root root C,4@7 a alpha, (,x,C,8 b beta,),x,C,9
-part2-cymene root root C,408 a alpha, (,x,C,9,),x,C,10
-part2-anisidine root root 0,4@x,C,a|alpha
-part2-thioanisidine root root S,4@x,C,a|alpha
-part2-phenetidine root root O,4@x,C,a|alpha,C,b|beta
-part2-xylidine root root C,4@a alpha
-part2-arsanil root root N,4@n
-part2-coumar root root 0,40x
indophenol root root
O, x, =, x, C, 1, Ring, Ring1, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, Ring, Ring1,), x, =, x, N, x, C,
1',Ring,Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ri
ng,Ring2
thymolindophenol root root
O, x, =, x, C, 1, Ring, Ring1, C, 2, =, x, C, 3, C, 4, (, x, C, 5, =, x, C, 6, Ring, Ring1,), x, =, x, N, x, C,
1',Ring,Ring2,=,x,C,2'|m|meta,C,3'|o|ortho,(,x,C,x,(,x,C,x,),x,C,x,),x,=,x,C,4',
(,x,0,x,),x,C,5',=,x,C,6',(,x,C,x,),x,Ring,Ring2
```

```
cresolindophenol root root
0,x,=,x,C,1,Ring,Ring1,C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6,Ring,Ring1,),x,=,x,N,x,C,
1', Ring, Ring2, =, x, C, 2' | m | meta, (C), x, C, 3' | 0 | ortho, =, x, C, 4', (, x, 0, x, ), x, C, 5', =, x, C
picoline|picolin|picol toluene picoline
c,2,Ring,Ring1,c,3|b|beta,c,4|g|gamma,c,5,c,6,n,1,Ring,Ring1
pipecoline | pipecolin | pipecol toluene picoline
C,2|a|alpha,Ring,Ring1,C,3|b|beta,C,4|g|gamma|p,C,5,C,6,N,1,Ring,Ring1
toluene tolu tol toluene toluene
c,1,Ring,Ring1,c,2|o|ortho,Ring,Ring2,.,x,c,4|p|para,Ring,Ring3,Ring,Ring4,.,x,c
,6,Ring,Ring5,Ring,Ring1,.,x,c,3|m|meta,Ring,Ring2,Ring,Ring3,.,x,c,5,Ring,Ring4
, Ring, Ring5
toluidide otoluidide toluide toluide toluidide toluene
0,8@x,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing, Ring1
cumidine cumidin toluene cumene
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cumene cumen toluene cumene
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cumyl|alphacumyl root root
C,4@a|alpha,(C)(C),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
cumidene cumiden toluene cumene
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cymene cymen toluene cymene
C,7|a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylene xylol toluene toluene
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylen xyl toluene xylidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidide oxylidide xylide oxylide toluidide xylidine
0,80x,.,x,N,40x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing, Ring1
anis toluene anisidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
thioanis toluene thioanisidine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
homoanis toluene anisidine
C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anisidide oanisidide aniside oaniside toluidide anisidine
0,8@x,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing, Ring1
anisal toluene anisidine
C,8@x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
mentha|menth|neomenth|neomentha|isomenth|isomentha toluene cymene
C,3 |m|meta, Ring, Ring1, C,4 |p|para, C,5, C,6, C,1, Ring, Ring2, C,2 |o|ortho, Ring, Ring1,.
x,C,7|a|alpha,Ring,Ring2
anisidine anisidin toluene anisidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anisidino toluene anisidine
N, 4@n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
phenetidine phenetidin toluene phenetidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
phenetidide ophenetidide phenetide ophenetide toluidide phenetidine
0,8@x,.,x,N,4@x,c,1',Ring,Ring1,c,2'|o|ortho,c,3'|m|meta,c,4'|p|para,c,5',c,6',R
ing,Ring1
phenetidino toluene phenetidine
N, 4@n, c, 1, Ring, Ring1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring1
```

```
cresyl toluene toluene
0,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring1
cres toluene toluene
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
thiocresol toluene toluene
S,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
cresylicacid toluene toluene
0,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
cresot toluene toluene
c, 2, Ring, Ring1, (0), x, c, 3 | o | ortho, c, 4 | m | meta, c, 5 | p | para, c, 6, c, 1, (, x, C, x,), x, Ring, c, 2, Ring, c, 2, Ring, c, 3, c, 4, c, 4, c, 5, c, 6, c, 1, c, 5, c, 6, c, 1, c, 7, c, 8, c, 7, c, 8, c, 1, c, 1, c, 8, c, 1, c, 1
Ring1
toluidine toluidin toluene toluene
N.n.c.1.Ring,Ring1.c.20oortho.c.3 mmeta,c.4 ppara,c.5,c.6,Ring,Ring1
toluidino toluene toluene
N,4@n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidine xylidin toluene xylidine
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
xylidino toluene xylidine
N,40n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
coumar toluene coumar
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c, 6, Ring, Ring1
arsanil toluene tolarsanil
c,4|p|para,c,5,c,6,Ring,Ring1
tosyl ptosyl root root
S,40x, (=0), x, (=0), x,c,x,Ring,Ring1,ccc,x,(,x,C,x,),x,cc,x,Ring,Ring1
tosylate|ptosylate|tosylat|ptosylat|tosilate|ptosilate|tosilat|ptosilat root
root 0,10x,S,x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
tosylamido root root
N,40x,S,x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(C)cc,x,Ring,Ring1
brosylate|brosylat|brosilate|brosilat root root
0,10x,S,x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
brosyl root root S,40x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(Br)cc,x,Ring,Ring1
closylate|closylat|closilate|closilat root root
0.10x, S, x, (=0), x, (=0), x, c, x, Ring, Ring1, ccc(Cl)cc, x, Ring, Ring1
closyl root root S,40x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(Cl)cc,x,Ring,Ring1
nosylate|nosylat|nosilate|nosilat root root
0,10x,S,x,(=0),x,(=0),x,c,x,Ring,Ring1,cc([N+](=0)[0-])ccc,x,Ring,Ring1
mesylate | mesylat root root 0,10x,S,x,(=0),x,(=0),x,C,x
esylate esylat root root 0,10x,S,x,(=0),x,(=0),x,C,x,C,x
pipsyl root root S,4@x,(=0),x,(=0),x,c,x,Ring,Ring1,ccc(I)cc,x,Ring,Ring1
methosulfate | methosulfat | metilsulfate | metilsulfat root root
0.10x, S, x, (=0), x, (=0), x, 0, x, C, x
ethosulfate|ethosulfat|etilsulfate|etilsulfat root root
0,10x,S,x,(=0),x,(=0),x,0,x,C,x,C,x
desyl root root C,x,(C(=0)c1ccccc1)c2ccccc2,x
isoniazide isoniazid root root
c, 2, Ring, Ring1, c, 3, c, 4, (,x, C, x, (,x, =, x, 0, x,), x, N, x, N, n,), x, c, 5, c, 6, n, 1, Ring, Ring
pheneth root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring
 ,Ring1
secpheneth root root
C,a|alpha,(,x,C,b|beta,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c, 6, Ring, Ring1
```

12

ľΨ

Ű

- 2

111

13

ı. £

```
neoph root root
C,a|alpha,C,b|beta,(C)(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5
,c,6,Ring,Ring1
amphetamine amphetamin root root
N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
5,c,6,Ring,Ring1
methamphetamine methamphetamin root root
C,x,N,n,C,a|alpha,(C),x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|par
a,c,5,c,6,Ring,Ring1
ammelide root root
N, n, c, 6, Ring, Ring1, n, 1, c, 2, (, x, 0, x, ), x, n, 3, c, 4, (, x, 0, x, ), x, n, 5, Ring, Ring1
phenate|phenat|phenoxide|phenoxid root root [0-
],x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
phen root phenyl
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
benzyne benzyn root root
C,1,Ring,Ring1,\#,x,C,2|o|ortho,C,3|m|meta,=,x,C,4|p|para,C,5,=,x,C,6,Ring,Ring1
benzal root root
C,8@a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
benzene benzen benzol root root
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
dewarbenzene root root C12C=CC1C=C2,x
benzeneoxid|benzeneoxide root root
C,1,Ring,Ring1,(,x,0,x,Ring,Ring2,),x,C,2,Ring,Ring2,C,3,=,x,C,4,C,5,=,x,C,6,Ring
g,Ring1
benzo-quinone benzo-quinon root root
C, 1, Ring, Ring1, (=0), x, C, 2 | o | ortho, =, x, C, 3 | m | meta, C, 4 | p | para, (=0), x, C, 5, =, x, C, 6, R
ing, Ring1
benzo-quinodimethane|benzo-quinodimethan root root
C, 1, Ring, Ring1, (=, x, C, 207,), x, C, 2 | o | ortho, =, x, C, 3 | m | meta, C, 4 | p | para, (=, x, C, 208,)
x,C,5,=,x,C,6,Ring,Ring1
toluquinone|ptoluquinone root root
C,1,Ring,Ring1,(=0),x,C,2|o|ortho,(C),x,=,x,C,3|m|meta,C,4|p|para,(=0),x,C,5,=,x
,C,6,Ring,Ring1
xyloquinone|pxyloquinone root root
C, 1, Ring, Ring1, (=0), x, C, 2 | o | ortho, (C), x, =, x, C, 3 | m | meta, C, 4 | p | para, (=0), x, C, 5, =, x
,C,6,(C),x,Ring,Ring1
duroquinone root root CC(C(C(C)=C1C)=0)=C(C1=0)C,x
thymoquinone root root O=C(C(C)=C1)C=C(C1=O)C(C)C,x
hemellitol root root
c,1,(C),x,Ring,Ring1,c,2|o|ortho,(C),x,c,3|m|meta,(C),x,c,4|p|para,c,5,c,6,Ring,
Ring1
benzo benzo benzo
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
acene acene acene c1ccccc1,x
aphene acene aphene c1ccccc1,x
mandel amygdal root root
C,x,C,x,(,x,0,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
g,Ring1
mesit root root
c,2|o| ortho, Ring, Ring1, c,3|m| meta, (,x,C,alpha1|alpha2|alpha,),x,c,4|p| para, c,5,(alpha1|alpha2|alpha,)
,x,C,alpha3|alpha4|alpha',),x,c,6,c,1,(,x,C,alpha5|alpha6|alpha'',),x,Ring,Ring1
mesitylene mesitylen root root
C,alpha1 alpha2 alpha,c,1,Ring,Ring1,c,2 oortho,c,3 meta,(,x,C,alpha3 alpha4
alpha',),x,c,4|p|para,c,5,(,x,C,alpha5|alpha6|alpha'',),x,c,6,Ring,Ring1
durene duren root root
C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met
```

```
a,c,4|p|para,(,x,C,a''|alpha''|alpha4,),x,c,5,(,x,C,a'''|alpha'''|alpha5,),x,c,6
,Ring,Ring1
isodurene isoduren root root
C,a|alpha|alpha1,c,1,Ring,Ring1,c,2|o|ortho,(,x,C,a'|alpha'|alpha2,),x,c,3|m|met
a, (x, C, a'' | alpha'' | alpha3,), x, c, 4 | p | para, c, 5, (x, C, a''' | alpha''' | alpha5,), x, c, 6
,Ring,Ring1
anisole anisol root root
C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
1
catechol root root
c,1,Ring,Ring1,(,x,0,o,),x,c,2|ortho,(,x,0,o',),x,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring, Ring1
phenetole|phenetol root root
C,b|beta,C,a|alpha,O,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring, Ring1
anethole anethol root root
C,x,0,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x,C,x,),x
,c,5,c,6,Ring,Ring1
dihydroanethole dihydroanethol root root
C,x,0,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x,),x,c,5
,c,6,Ring,Ring1
guaiacol root root
C,x,0,x,c,2 o ortho,Ring,Ring1,c,1,(,x,0,x,),x,c,6,c,5,c,4 p para,c,3 m meta,Rin
g,Ring1
quaiacolate root root
C,x,0,x,c,2|o|ortho,Ring,Ring1,c,1,(,x,0,1@x,),x,c,6,c,5,c,4|p|para,c,3|m|meta,R
ing,Ring1
veratrole veratrol root root
C,x,0,x,c,1,Ring,Ring1,c,2|o|ortho,(,x,0,x,C,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
eugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,0,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,=,x
(C,x,),x,c,5,c,6,Ring,Ring1
dihydroeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,0,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,C,x,C,x
,),x,c,5,c,6,Ring,Ring1
isoeugen root root
c,1,Ring,Ring1,c,2|o|ortho,(,x,0,x,C,x,),x,c,3|m|meta,c,4|p|para,(,x,C,x,=,x,C,x
(C,x,),x,c,5,c,6,Ring,Ring1
isoeugenol root root
(C,x,C,x,),x,c,5,c,6,Ring,Ring1
styr|styrene|styren|styrol|cinnamene|cinnamenol|cinnamol root root
C,b|beta|w|omega,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,
c,5,c,6,Ring,Ring1
styrall|styral root root
C,b|beta,(,x,C,a|alpha,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c, 6, Ring, Ring1
phosphinine root root
p,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anthranil root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,(,x,N,n,),x,c,3|m|meta,c,4|p|para,c,5,c,6,R
ing,Ring1
hippur root trivial
C,x,C,x,N,x,C,x,(,x,=,x,0,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para
,c,5,c,6,Ring,Ring1
```

```
carbanil loveracid root
C,x,N,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
shikim root root
C, x, C, 1, Ring, Ring1, =, x, C, 2, C, 3, (0), x, C, 4, (0), x, C, 5, (0), x, C, 6, Ring, Ring1
benzo|benz|dracyl root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
crithmin root root
nq1
C, a | alpha, c, 1, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5, c, 6, Ring, Ring 1, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5 | ortho, c, 3 | m | meta, c, 4 | p | para, (OC), x, c, 5 | ortho, c, 5 | o
ing1
vanill root root
(x,),x,c,5,c,6,Ring,Ring1
isovanill root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(0),x,c,4|p|para,(0C),x,c,5,c,6,
Ring, Ring1
homovanill root root
C,a|alpha,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,),x,c,4|p|para,(
(x,0,x,),x,c,5,c,6,Ring,Ring1
vanillin root root
0,x,Ring,Ring2,..,x,0,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),
x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
ethylvanillin root root
0,x,Ring,Ring2,.,x,0,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OCC)
 x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
isovanillin root root
0,x,Ring,Ring2,..,x,0,x,=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,Ring,
Ring2,c,4|p|para,(OC),x,c,5,c,6,Ring,Ring1
acetovanillone root root
0,x,=,x,C,a|alpha,(C),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,),x,c,
4|p|para, (,x,0,x,),x,c,5,c,6,Ring,Ring1
safrole safrol root root
C,x,=,x,C,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,0,x,Ring,Ring2)
 ,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
dihydrosafrole|dihydrosafrol root root
C,x,C,x,C,x,c,1, Ring, Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,0,x,Ring,Ring2,),x
 ,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 isosafrole isosafrol root root
C,x,C,x,=,x,C,x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,0,x,Ring,Ring2)
 ,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
piperon root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,0,x,Ring,Ring2,),x,c
 ,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
homopiperon root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,C,x,0,x,Ring,Ri
ng2,),x,c,4|p|para,Ring,Ring2,c,5,c,6,Ring,Ring1
 veratr root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),x,c,5,c,6
 ,Ring,Ring1
homoveratr root root
 C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|para,(OC),
 x,c,5,c,6,Ring,Ring1
 protocatechu root root
 C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,),x,c,4|p|para,(,x,0,x,)
 x,c,5,c,6,Ring,Ring1
```

```
homoprotocatechu root root
C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,),x,c,4|p|para,
(,x,0,x,),x,c,5,c,6,Ring,Ring1
citrazin root root
(x,),x,c,6,Ring,Ring1
gall root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(,x,0,x,),x,c,4|p|para,(,x,0,x,)
x,c,5,(,x,0,x,),x,c,6,Ring,Ring1
gallacetophenone root root O=C(C)C1=C(O)C(O)=C(O)C=C1, x
toluene toluol root root
C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,=,x,c,6,Ring,Ring
cumene cumen root root
C,x,C,a|alpha,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c
,6,Ring,Ring1
aniline anilin analine analin root root
N,n,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anilino analino root root
N, 4@n, c, 1, Ring, Ring1, c, 2 o ortho, c, 3 m meta, c, 4 p para, c, 5, c, 6, Ring, Ring1
gentis root root
C,x,c,1,Ring,Ring1,c,2,(,x,0,o,),x,c,3|m|meta,c,4|p|para,c,5,(,x,0,o',),x,c,6,Ri
ng, Ring1
homogentis root root
C,x,C,x,c,1,Ring,Ring1,c,2,(,x,0,0,),x,c,3|m|meta,c,4|p|para,c,5,(,x,0,0',),x,c,
6, Ring, Ring1
salicyl|salic root root
\texttt{C,x,c,1,Ring,Ring1,c,2,(,x,0,o,),x,c,3} \\ | \texttt{m}| \texttt{meta,c,4} \\ | \texttt{p}| \texttt{para,c,5,c,6,Ring,Ring1} \\ | \texttt{meta,c,4}| \texttt{p}| \texttt{para,c,5,c,6,Ring,Ring1} \\ | \texttt{meta,c,6}| \texttt{para,c,6,Ring,Ring1} \\ | \texttt{meta,c,6}| \texttt{para,c,6,Ring,Ring1} \\ | \texttt{para,c,6,Ring,Ring1}| \texttt{para,c,6,Ring1} \\ | \texttt{para,c,6,Ring1}| \texttt{para,c,6,Ring1} \\ |
salicylal root root
C,8@x,c,1,Ring,Ring1,c,2,(,x,0,0,),x,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
anilot root root
C,x,c,1,Ring,Ring1,c,2,(,x,0,0,),x,c,3|m|meta,c,4|p|para,c,5,([N+](=0)[0-1])
]),x,c,6,Ring,Ring1
alpharesorcyl aresorcyl root root
C,x,c,1,Ring,Ring1,c,2,c,3|m|meta,(,x,0,x,),x,c,4|p|para,c,5,(,x,0,x,),x,c,6,Rin
g,Ring1
betaresorcyl|bresorcyl root root
C,x,c,1,Ring,Ring1,c,2,(,x,0,x,),x,c,3|m|meta,c,4|p|para,(,x,0,x,),x,c,5,c,6,Rin
gammaresorcyl gresorcyl root root
C,x,c,1,Ring,Ring1,c,2,(,x,0,x,),x,c,3|m|meta,c,4|p|para,c,5,c,6,(,x,0,x,),x,Rin
g,Ring1
phenac root root
C,a|alpha,C,x,(,x,=,x,0,x,),x,c,x,Ring,Ring1,=,x,c,2|o|ortho,c,3|m|meta,c,4|p|pa
ra,c,5,c,6,Ring,Ring1
 trop root root
C,x,C,x,(,x,C,x,0,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
 ,Ring,Ring1
nortrop root root
\texttt{C,x,(,x,C,x,0,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin}
q,Ring1
hydratrop root root
 C,x,C,x,(,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Rin
homatrop root root CN1C2CCC1CC(OC(C(0)C3=CC=CC=C3)=O)C2,x
 atrop root root OCC(C(OC3CC2CCC(C3)N2C)=O)c1ccccc1,x
```

```
tropan tropane root root C,3,(,x,C,2,C,1,Ring,Ring1,Ring,Ring2,),x,C,4,C,5 a-
r, (x, C, 6 \mid a-b, C, 7 \mid a-t, Ring, Ring2,), x, N, 8, Ring, Ring1, C, x
tropin|tropine root root C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,(0),x,C,4,C,5|a-
r, (x, C, 6 \mid a-b, C, 7 \mid a-t, Ring, Ring2,), x, N, 8, Ring, Ring1, C, x
1alphah5alphahtropan root root
C,3,(x,C,2,[C@],1,([H]),x,Ring,Ring1,Ring,Ring2,),x,C,4,[C@],5|a-
r,([H]),x,(,x,C,6|a-b,C,7|a-t,Ring,Ring2,),x,N,8,Ring,Ring1,C,x
tropinone root root CN1C(C2)CCC1CC2=0,x
atrolact root root
C,x,C(C)(O),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring
cinnamo cinnam root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,
c, 6, Ring, Ring1
cinnamal root root
C,80x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,
5,c,6,Ring,Ring1
hydrocinnam root root
C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,
Ring, Ring1
hydrocinnamal root root
C,80x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,c,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,c,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,c,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,a|alpha,c,b|beta,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alpha,c,5|alp
6, Ring, Ring1
grevill root root
C,x,/,x,C,a|alpha,=,x,C,b|beta,/,x,c,1,Ring,Ring1,c,2|o|ortho,(0),x,c,3|m|meta,c
,4|p|para,c,5,(0),x,c,6,Ring,Ring1
caffe root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(0),x,c,4|p|par
a, (0), x, c, 5, c, 6, Ring, Ring1
ferul root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra, (0), x, c, 5, c, 6, Ring, Ring1
sinap root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra, (0), x, c, 5, (0C), x, c, 6, Ring, Ring1
conifer | conifero root root
C,x,C,a|alpha,=,x,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,(OC),x,c,4|p|pa
ra, (0), x, c, 5, c, 6, Ring, Ring1
phloret root root
C,x,C,a|alpha,C,b|beta,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,(0),x,c,
5,c,6,Ring,Ring1
nicotino nicotine nicotin loveracid root
C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
nicotin root root C,x,c,3,Ring,Ring1,c,4,c,5,c,6,n,1,c,2,Ring,Ring1
isonicotino isonicotin root root
c,x,c,4,Ring,Ring1,c,5,c,6,n,1,c,2|a|alpha,c,3|b|beta,Ring,Ring1
melamine melamin root root
n, 1, Ring, Ring1, c, 2, (N), x, n, 3, c, 4, (N), x, n, 5, c, 6, (N), x, Ring, Ring1
pyrylium root root
[o+],1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
naphtho|naphth|naphthalene|naphthalen root root
\verb|c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8|
,c,8a|8alpha,Ring,Ring1,Ring,Ring2
naphtho naphth opfuser unknown
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8
,c,8a|8alpha,Ring,Ring1,Ring,Ring2
```

```
naphtho-quinone|naphtho-quinon|naphthalene-quinone|naphthalene-quinon root root
c,1|a|alpha,(=0),x,Ring,Ring1,c,2|b|beta,=,x,c,3,c,4,(=0),x,c,4a|4alpha,Ring,Rin
g2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
cadalene cadalen root root
c,1|a|alpha,(C),x,Ring,Ring1,c,2|b|beta,c,3,c,4,(C(C)C),x,c,4a|4alpha,Ring,Ring2
,c,5,c,6,(C),x,c,7,c,8,c,8a|8alpha,Ring,Ring1,Ring,Ring2
benzodioxene benzodioxen root root
o,1,Ring,Ring1,c,2,c,3,o,4,c,4a|4alpha,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a|8alpha,Ri
ng, Ring1, Ring, Ring2
azulene azulen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
azuleno azulen opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
anthracene anthracen anthro anthr root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Rin
g3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
anthrone anthron root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,C,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,C,9,(=,x,0,x,),x,c,9a,Ring,Ring2,Ring,Ring1
anthra-quinone|anthra-quinon|anthracene-quinone|anthracene-quinon root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,C,10,(=0),x,c,5a|10a,R
ing, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring2, Ring, Ring2, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring2, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring, Ring3, C, 9, (=, x, 0, x,), x, c, 9a, Ring3, C, 
Ring1
anthra anthraceno opfuser unknown
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,10,c,5a|10a,Ring,Ring
q3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
acrid root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,c,9a,Ring,Ring2,Ring,Ring1
aminacrine aminacrin aminacridin aminacridine monacrin monacrine root root
c,1|a|alpha,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,n,10,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,9,(N),n,c,9a,Ring,Ring2,Ring,Ring1
acenaphthene acenaphthen root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
acenaphtho acenaphth opfuser unknown
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
acenaphthylene|acenaphthylen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring, Ring1, c, 8b, Ring, Ring2, Ring, Ring3
cholanthrene cholanthren root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,6b,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,12,c,12a,Ring,Ring4,
c,12b,Ring,Ring1,c,12c,Ring,Ring3,Ring,Ring2
phenalene phenalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
 ,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3
 julolid root root
C,1,Ring,Ring1,C,2,c,C,N,4,Ring,Ring2,C,5,C,6,C,7,c,7a,Ring,Ring3,c,8,c,9,c,10,c
 ,10a,Ring,Ring1,c,10b,Ring,Ring2,Ring,Ring3
perimid root root
n,1,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
```

,9a,Ring,Ring1,c,9b,Ring,Ring2,Ring,Ring3

```
phenanthren phenanthrene root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, c, 9, c, 10, c, 10a, Ring, Ring1, Ring, Ring2
phenanthr|phenanthro|phenanthra opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, c, 9, c, 10, c, 10a, Ring, Ring1, Ring, Ring2
cyclopentadefphenanthren|cyclopentadefphenanthrene root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,4a,Ring,Ring3,c,5,c,6,c,7,c,7a,Ring
,Ring4,c,8,c,9,c,8a,Ring,Ring1,c,8b,Ring,Ring2,c,8c,Ring,Ring3,Ring,Ring4
bathophenanthroline root root
n,1,Ring,Ring1,c,2,c,3,c,4,(c4cccc4),x,c,4a,Ring,Ring2,c,5,c,6,c,6a,Ring,Ring3,
c,7,(c5cccc5),x,c,8,c,9,n,10,c,10a,Ring,Ring3,c,10b,Ring,Ring1,Ring,Ring2
phenanthrone phenanthron root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, C, 9, (=0), x, C, 10, c, 10a, Ring, Ring1, Ring, Ring2
phenanthrene-quinone|phenanthrene-quinon root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, c, 9, (=0), x, c, 10, (=0), x, c, 10a, Ring, Ring1, Ring2
cyclopentaaphenanthrene cyclopentaaphenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,c,14,Ring,Ring4
,c,15,c,16,c,17,c,13,Ring,Ring4,c,12,c,11,c,9,Ring,Ring3,c,10,Ring,Ring2,Ring,Ri
nq1
fluoranthene|fluoranth|fluoranthen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
acephenanthrene acephenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,ring2,C,4,C,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
acephenanthrylene acephenanthrylen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
aceanthrene aceanthren root root
C,1,Ring,Ring1,C,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
aceanthrylene aceanthrylen root root
 c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Rin
 g4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring1,c,10c,Ring,Ring2,Ring,Ring
 3
 violanthrene violanthren root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,c,5a,Ring,Ring3,c,6,c,7,c,7a,Ring
 , Ring4, c, 7b, Ring, Ring5, c, 8, c, 9, c, 9a, (, x, c, 18f, Ring, Ring6, c, 18e, Ring, Ring7, Ring, Ring6, c, 18e, Ring, Ring7, Ring6, Rin
 ing5,),x,C,10,c,10a,Ring,Ring8,c,11,c,12,c,13,c,14,c,14a,Ring,Ring8,c,14b,Ring,R
 ing6,c,15,c,16,c,16a,Ring,Ring7,c,16b,Ring,Ring9,c,17,c,18,c,18a,(,x,c,18b,Ring,
 Ring1, Ring, Ring2, ), x, c, 18c, Ring, Ring3, c, 18d, Ring, Ring4, Ring, Ring9
 isoviolanthrene|isoviolanthren root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,6a,(,x,c,18
 c,Ring,Ring4,c,18b,Ring,Ring5,Ring,Ring3,),x,c,6b,Ring,Ring6,c,7,c,8,c,8a,(,x,c,
 18e, Ring, Ring7, c, 18d, Ring, Ring8, Ring, Ring6, ), x, C, 9, c, 9a, Ring, Ring9, c, 10, c, 11, c, 1
 2,c,13,c,13a,Ring,Ring9,c,13b,Ring,Ring7,c,14,c,15,c,15a,Ring,Ring8,c,15b,Ring,R
 ing4,c,16,c,17,c,17a,Ring,Ring5,C,18,c,18a,Ring,Ring1,Ring,Ring2
 triphenylene triphenylen root root
 c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
```





Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring2,Ring,Ring1

trindene trinden root root

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Ring4,c,7,c,8,c,9,c,9a,Ring,Ring4,c,9b,Ring,Ring2,Ring,Ring1 pyrene | pyren root root

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,Ring,Ring4,c,9,c,10,c,10a,Ring,Ring1,c,10b,Ring,Ring2,c,10c,Ring,Ring3,Ring,Ring

chrysene chrysen root root

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,6a,Ring,Ring4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,10b,Ring,Ring3,c,11,c,12,c,12a,Ring,Ring2,Ring,Ring1

naphthacene naphthacen root root

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Ring4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2,Ring,Ring1

naphthaceno naphthacen opfuser unknown

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,6,c,6a,Ring,Ring4,c,7,c,8,c,9,c,10,c,10a,Ring,Ring4,c,11,c,11a,Ring,Ring3,c,12,c,12a,Ring,Ring2,Ring,Ring1

pleiadene pleiaden root root

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,7,c,7a,Ring,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,12,c,12a,Ring,Ring1,c,12b,Ring,Ring3,Ring,Ring2

picene|picen root root

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Ring4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,11,c,12,c,12a,Ring,Ring5,c,12b,Ring,Ring4,c,13,c,14,c,14a,Ring,Ring3,c,14b,Ring,Ring2,Ring,Ring1

perylene perylen root root

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Ring
g4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ring4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring3

perylo opfuser unknown

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring3,c,6b,Ring,Ring4,c,7,c,8,c,9,c,9a,Ring,Ring5,c,10,c,11,c,12,c,12a,(,x,c,12d,Ring,Ring5,Ring,Ring4,),x,c,12b,Ring,Ring1,c,12c,Ring,Ring2,Ring,Ring3

tetraphenylene tetraphenylen root root

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,c,8b,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,c,12b,Ring,Ring5,c,13,c,14,c,15,c,16,c,16a,Ring,Ring5,c,16b,Ring,Ring2,Ring,Ring1 rubicene root root

c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,3b,Ring,Ring3,c,4,c,5,c,6,c,7,c,7a,Ring,Ring3,c,7b,Ring,Ring4,c,7c,Ring,Ring5,c,8,c,9,c,10,c,10a,Ring,Ring6,c,10b,Ring,Ring7,c,11,c,12,c,13,c,14,c,14a,Ring,Ring7,c,14b,(,x,c,14e,Ring,Ring6,Ring,Ring5,),x,c,14c,Ring,Ring1,c,14d,Ring,Ring2,Ring,Ring4

coronene coronen root root

c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,4a,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
g4,c,7,c,8,c,8a,Ring,Ring5,c,9,c,10,c,10a,Ring,Ring6,c,11,c,12,c,12a,Ring,Ring1,
c,12b,Ring,Ring7,c,12c,Ring,Ring2,c,12d,Ring,Ring3,c,12e,Ring,Ring4,c,12f,Ring,R
ing5,c,12g,Ring,Ring6,Ring,Ring7

trinaphthylene trinaphthylen root root

c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5,c,5a,Ring,Ring3,c,5b,Ring,Ring4,c
,6,c,6a,Ring,Ring5,c,7,c,8,c,9,c,10,c,10a,Ring,Ring5,c,11,c,11a,Ring,Ring4,c,11b
,Ring,Ring6,c,12,c,12a,Ring,Ring7,c,13,c,14,c,15,c,16,c,16a,Ring,Ring7,c,17,c,17
a,Ring,Ring6,c,17b,Ring,Ring3,c,18,c,18a,Ring,Ring2,Ring,Ring1

ing, Ring2, o, 1, Ring, Ring1

```
pyranthrene pyranthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,5a,Ring,Ring4,c
,6,c,7,c,7a,Ring,Ring5,c,8,c,8a,Ring,Ring6,c,9,c,10,c,11,c,12,c,12a,Ring,Ring6,c
,12b,Ring,Ring7,c,13,c,13a,Ring,Ring8,c,14,c,15,c,15a,(,x,c,16,c,16a,Ring,Ring2,
Ring, Ring1,),x,c,15b,Ring,Ring3,c,15c,Ring,Ring8,c,15d,Ring,Ring4,c,15e,Ring,Rin
g7,Ring,Ring5
ovalene ovalen root root
c,1,Ring,Ring1,c,2,c,2a,Ring,Ring2,c,3,c,4,c,4a,Ring,Ring3,c,5,c,6,c,6a,Ring,Rin
g4,c,7,c,7a,Ring,Ring5,c,8,c,9,c,9a,Ring,Ring6,c,10,c,11,c,11a,Ring,Ring7,c,12,c
,13,c,13a,Ring,Ring8,c,14,c,14a,Ring,Ring1,c,14b,Ring,Ring9,c,14c,Ring,Ring2,c,1
4d, Ring, Ring3, c, 14e, Ring, Ring4, c, 14f, Ring, Ring0, c, 14g, Ring, Ring5, c, 14h, Ring, Ring
6,c,14i,Ring,Ring7,c,14j,Ring,Ring8,c,14k,Ring,Ring0,Ring9,Ring9
biphenylene biphenylen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, c, 8b, Ring, Ring2, Ring, Ring1
thianthrene thianthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,s,10,c,10a,Ring,Ring2,Ring,Ring1
pyr root root
c,2|a|alpha,Ring,Ring1,c,3|b|beta,c,4|g|gamma,c,5,c,6,o,1,Ring,Ring1
pyrano opfuser unknown c,2,Ring,Ring1,c,3,c,4,c,5,c,6,o,1,Ring,Ring1
mdioxine mdioxin root root c,2,Ring,Ring1,o,3,c,4,c,5,c,6,o,1,Ring,Ring1
pdioxine|pdioxin root root c,2,Ring,Ring1,c,3,o,4,c,5,c,6,o,1,Ring,Ring1
oxalene oxalen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, o, 7, c, 7a, Ring, Ring2, Ring, Ring
azalene azalen root root
c, 1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, n, 7, c, 7a, Ring, Ring2, Ring, Ring
isobenzofuran root root
c,1,Ring,Ring1,o,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
benzofurazan root root
n,1,Ring,Ring1,o,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
benzofuroxan root root [n+],1,(,x,[0-
[,x,),x,Ring,Ring1,o,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,
Ring1
piazthiole root root
n,1,Ring,Ring1,s,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ring,Ring
catecholborane root root
o,x,Ring,Ring1,B,b,O,x,c,2,Ring,Ring2,c,3,c,4,c,5,c,6,c,1,Ring,Ring2,Ring,Ring1
chromene chromen root root
c, 2, Ring, Ring1, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, o, 1, Ring,
Ring1
chromane chroman root root
C,2,Ring,Ring1,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,
Ring1
chromone chromon root root
c,2,Ring,Ring1,c,3,c,4,(=0),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,
1, Ring, Ring1
esculetin root root
c, 2, Ring, Ring1, (=0), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, (0), x, c, 7, (0), x, c, 8, c, 8a, R
```

```
umbelliferone root root
c,2,Ring,Ring1,(=0),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,(0),x,c,8,c,8a,Ring,Ri
ng2,o,1,Ring,Ring1
umbelliferyl root root
c,2,Ring,Ring1,(=0),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,4@7,c,8,c,8a,Ring,Ring2,
o,1,Ring,Ring1
isochromane isochroman root root
C,1,Ring,Ring1,O,2,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,
Ring2
flav root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,C,4|a-
1,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,0,1,Ring,Ring1,),x,c,1',Ring,R
ing3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
flavone|flavon root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1, (=0), x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1'
 Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
acacetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(OC),x,c,5',c,6',Ring,Ring3
alpinetin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-
1, (=0), x,c, 4a, Ring, Ring2,c,5, (OC), x,c,6,c,7, (O), x,c,8,c,8a, Ring, Ring2,o,1, Ring, R
ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
apigenin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
1, (=0), x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3
baicalein root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 l, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,(0),x,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,R
 ing,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
catechin root root C,2|a-t,(x,Ring,Ring1,C,3|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C,4|a-b,(0),x,C
 1,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,0,1,Ring,Ring1,),x
 ,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',c,6',Ring,Ring3
chrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3
cirsiliol root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0), x, c, 4a, Ring, Ring2, c, 5, (0), x, c, 6, (0C), x, c, 7, (0C), x, c, 8, c, 8a, Ring, Ring2, o, 1
 Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (0), x, c, 4', (0), x, c, 5', c, 6', Ring, Ring3
diosmetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
ng1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0C),x,c,5',c,6',Ring,Ring3
 epicatechin root root C, 2|a-t, (x, Ring, Ring1, C, 3|a-b, (0), x, C, 4|a-b, (0), 
 1,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x
 ,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',c,6',Ring,Ring3
 eupatorin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0), x, c, 4a, Ring, Ring2, c, 5, (0), x, c, 6, (0C), x, c, 7, (0C), x, c, 8, c, 8a, Ring, Ring2, o, 1
 , Ring, Ring1,), x,c,1', Ring, Ring3,c,2',c,3',(0),x,c,4',(0C),x,c,5',c,6', Ring, Ring3
 galangin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c
 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3
 genkwanin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0), x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0C),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R
 ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3
 hesperitin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-
 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 ng1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0C),x,c,5',c,6',Ring,Ring3
 kaempferide | kaempferol root root c,2 | a-t,(,x,Ring,Ring1,c,3 | a-b,(0),x,c,4 | a-
 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri
 nq1,),x,c,1',Rinq,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3
```





luteolin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-1, (=0), x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri ng1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',c,6',Ring,Ring3 morin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri ng1,),x,c,1',Ring,Ring3,c,2',(0),x,c,3',c,4',(0),x,c,5',c,6',Ring,Ring3 myricetin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,1, (=0), x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri ng1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',(0),x,c,6',Ring,Ring3 naringenin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-1, (=0), x, c, 4a, Ring, Ring, c, 5, (0), x, c, 6, c, 7, (0), x, c, 8, c, 8a, Ring, Ringng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3 pinocembrin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-1, (=0), x, c, 4a, Ring, Ring2, c, 5, (0), x, c, 6, c, 7, (0), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ri ng1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3 pinostrobin root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,c,4|a-1, (=0), x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0C),x,c,8,c,8a,Ring,Ring2,o,1,Ring,R ing1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3 quercetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri ng1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',c,6',Ring,Ring3 robinetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x1, (=0), x,c,4a,Ring,Ring2,c,5,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,), x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',(0),x,c,6',Ring,Ring3 sinensetin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-1, (=0), x, c, 4a, Ring, Ring, 2, c, 5, (OC), x, c, 6, (OC), x, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring, 2, o, and a simple of the second sec1,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(OC),x,c,5',c,6',Ring,Rin syringetin root root $c, 2 \mid a-t, (x, Ring, Ring, c, 3 \mid a-b, (0), x, c, 4 \mid a-b, (0)$ 1, (=0),x,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ri ng1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3 tectochrysin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|a-1, (=0), x, c, 4a, Ring, Ring, 2, c, 5, (0), x, c, 6, c, 7, (0C), x, c, 8, c, 8a, Ring, Ring, 2, c, 1, Ring, Rining1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3 isoflavone|isoflavon root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-1, (=0), x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,),x,c,1' Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3 daidzein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-1, (=0), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, (0), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3 formononetin root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-1, (=0), x,c,4a,Ring,Ring2,c,5,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,o,1,Ring,Ring1,), x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3 genistein root root c,2|a-t,Ring,Ring1,c,3|a-b,(,x,c,4|a-1, (=0), x, c, 4a, Ring, Ring2, c, 5, (0), x, c, 6, c, 7, (0), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1,),x,c,1',Ring,Ring3,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring3 flavylium root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,c,4|al,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,),x,c,1',Rin g,Ring3,c,2',c,3',c,4',c,5',c,6',Ring,Ring3 malvidin root root c,2|a-t,(x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,c,4|a-b,(0),x,cl,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(OC),x,c,4',(O),x,c,5',(OC),x,c,6',Ring,Ring3 cyanidin root root c,2|a-t,(,x,Ring,Ring1,c,3|a-b,(0),x,c,4|a-1,c,4a,Ring,Ring2,c,5,(0),x,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring2,[o+],1,Ring,Ring1,),x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(0),x,c,5',c,6',Ring,Ring3

```
flavanone|flavanon root root C,2|a-t,(,x,Ring,Ring1,C,3|a-b,C,4|a-
1, (=0), x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring2,O,1,Ring,Ring1,),x,c,1'
Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
anaphthoflavone anaphthoflavon alphanaphthoflavone alphanaphthoflavon root root
O=C2C=C(C4=CC=CC=C4)OC1=C3C(C=CC=C3)=CC=C12,x
bnaphthoflavone|bnaphthoflavon|betanaphthoflavone|betanaphthoflavon root root
O=C2C=C(C3=CC=CC=C3)OC1=CC=C4C(C=CC=C4)=C12,x
xanthene | xanthen | xanthydr | xanth root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ring,R
ing3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
xanthone xanthon root root
c,9,Ring,Ring1,(,x,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,10,c,10a,Ri
ng,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1,),x,=0,x
xanthylium root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[o+],10,c,10a,Rin
g, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, Ring, Ring1
xanthuren root root
C,x,c,2,Ring,Ring1,c,3,c,4,(0),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(0),x,c,8a,Ring
,Ring2,n,1,Ring,Ring1
thioxanthene thioxanthen root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,10,c,10a,Ring,R
ing3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
selenoxanthene selenoxanthen root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],10,c,10a,Rin
q,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
acridars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,c,10,c,10a,Ring,Ring2,Ring,Ring1
arsanthrene arsanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phosphanthrene phosphanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,p,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,p,10,c,10a,Ring,Ring2,Ring,Ring1
selenanthrene selenanthren root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[se],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[se],10,c,10a,Ring,Ring2,Ring,Ring1
phenomercurin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Hg],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,[Hg],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxathiin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,s,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxastannin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxagermanin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,O,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Ge],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiastannin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
```

,9a,Ring,Ring3,[Sn],10,c,10a,Ring,Ring2,Ring,Ring1

```
phenothiasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiagermanin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,S,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Ge],10,c,10a,Ring,Ring2,Ring,Ring1
phenaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
phenazasiline|phenazasilin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,N,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Si],10,c,10a,Ring,Ring2,Ring,Ring1
phenarsaz phenoarsaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenothiaz thiodiphenylamine root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
phenomercaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,N,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Hg],10,c,10a,Ring,Ring2,Ring,Ring1
phenophosphaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,p,10,c,10a,Ring,Ring2,Ring,Ring1
phenotelluraz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Te],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,N,10,c,10a,Ring,Ring2,Ring,Ring1
phenoselenaz root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[Se],5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,
9,c,9a,Ring,Ring3,N,10,c,10a,Ring,Ring2,Ring,Ring1
phenothiars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,s,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxantimon root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,0,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Sb],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxars root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[as],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaphos root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,0,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,P,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxatellur root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,0,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Te],10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaselen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,0,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,[Se],10,c,10a,Ring,Ring2,Ring,Ring1
dibenzodioxin root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,o,10,c,10a,Ring,Ring2,Ring,Ring1
phenoxaz phenazox root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,o,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,n,10,c,10a,Ring,Ring2,Ring,Ring1
indene | inden root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
```

```
indeno opfuser unknown
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
indole | indol root root
n,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
thianaphthene|thianaphthen|thionaphthene|thionaphthen root root
s,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
thianaphtheno|thianaphthen opfuser unknown
s,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
isothianaphthene isothianaphthen root root
c,1,Ring,Ring1,s,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
isothianaphtheno|isothianaphthen opfuser unknown
c,1,Ring,Ring1,s,2|a|alpha,c,3|b|beta,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
skatole skatol root root
n,1,Ring,Ring1,c,2,c,3,(C),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Rin
g,Ring2
gramine root root
n,1,Ring,Ring1,c,2,c,3,(CN(C)C),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
1, Ring, Ring2
indolo opfuser unknown
n,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
isoindole isoindol root root
c,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
isoindolo opfuser unknown
c,1,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
arsindole arsindol root root
[as],1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
arsindolo opfuser unknown
[as],1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
isoarsindole|isoarsindol root root
c,1,Ring,Ring1,[as],2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
isoarsindolo|isoarsindol opfuser unknown
c,1,Ring,Ring1,[as],2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,R
ing2
phosphindole arsindol root root
p,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
phosphindolo|arsindol opfuser unknown
p,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
isophosphindole|isoarsindol root root
c,1,Ring,Ring1,p,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
isophosphindolo|isoarsindol opfuser unknown
c,1,Ring,Ring1,p,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
```

```
indazole indazol root root
n, 1, Ring, Ring1, n, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring
indazolo|indazol opfuser unknown
n, 1, Ring, Ring1, n, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring
indolizine indolizin pyrrocol root root
c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
indolizino opfuser unknown
c,1,Ring,Ring1,c,2,c,3,n,4,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
oxindole oxindol root root
N, 1, Ring, Ring1, C, 2, (=, x, 0, x, ), x, C, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ri
ng1,Ring,Ring2
indoline indolin root root
N,1,Ring,Ring1,C,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
isat root root
N,1,Ring,Ring1,C,2|alpha,(=0),x,C,3|beta,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,
c,7a,Ring,Ring1,Ring,Ring2
isoindoline isoindolin root root
C,1,Ring,Ring1,N,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
indane|indan|hydrindene|hydrind root root
C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring1, Ring, Ring2
hydrindantin root root 0=C(c2c1cccc2)C(C1=0)(0)C(C3=0)(0)C(c4c3cccc4)=0,x
alloxantin root root OC1(C2(C(NC(NC2=0)=0)=0)=0))O(NC(NC1=0)=0)=0, x
ninhydrin root root
C,1,(=0),x,Ring,Ring1,C,2,(=0),x,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a
,Ring,Ring1,Ring,Ring2
tetral root root
C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
decal root root
C,1|a|alpha,Ring,Ring1,C,2|b|beta,C,3,C,4,C,10,Ring,Ring2,C,5,C,6,C,7,C,8,C,9,Ri
ng, Ring1, Ring, Ring2
hexalin root root C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
quinol|chinol|quinolin|chinolin|leucol root root
n, 1, Ring, Ring1, c, 2|b|beta, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring
1, Ring, Ring2
quinolin chinolin opfuser unknown
n,1,Rinq,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
carbostyril|carbostyryl root root
n,1,Ring,Ring1,c,2|b|beta,(0),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2
isocarbostyril|isocarbostyryl root root
c,1,(0),x,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g, Ring1, Ring, Ring2
lepid root root
n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,(C),x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
g,Ring1,Ring,Ring2
cinchonin loveracid root
c,4,Ring,Ring1,c,3,c,2,n,1,c,8a,Ring,Ring2,c,8,c,7,c,6,c,5,c,4a,Ring,Ring1,Ring,
Ring2
```

```
quino chino opfuser unknown
n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
quinald chinald root root
C,a|alpha,Ring,Ring3,.,x,n,1,Ring,Ring1,c,2|b|beta,Ring,Ring3,c,3,c,4,c,4a,Ring,
Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring1,Ring,Ring2
xanthur root root
C,a|alpha,Ring,Ring3,...,x,n,1,Ring,Ring1,c,2|b|beta,Ring,Ring3,c,3,c,4,(0),x,c,4a
,Ring,Ring2,c,5,c,6,c,7,c,8,(0),x,c,8a,Ring,Ring1,Ring,Ring2
quinoliz chinoliz root root
c,1,Ring,Ring1,c,2,c,3,c,4,n,5,Ring,Ring2,c,6,c,7,c,8,c,9,c,8a,Ring,Ring2,Ring,R
ing1
quinazol chinazol root root
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
quinazol|chinazol|quinazolino opfuser unknown
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
isoquinol|isochinol root root
c,1|a|alpha,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing, Ring1, Ring, Ring2
isoquino isochino opfuser unknown
c,1|a|alpha,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing, Ring1, Ring, Ring2
cinnol root root
n,1,Ring,Ring1,n,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
quinoxal|chinoxal|phenpiaz root root
n,1,Ring,Ring1,c,2|b|beta,c,3,n,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
arsinol root root
[as],1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,R
ing1,Ring,Ring2
isoarsinol root root
c,1|a|alpha,Ring,Ring1,[as],2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8
a, Ring, Ring1, Ring, Ring2
phosphinol root root
p,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
1, Ring, Ring2
isophosphiol root root
c,1|a|alpha,Ring,Ring1,p,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
pterid root root
n,1,Ring,Ring1,c,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,n,5,c,6,c,7,n,8,c,8a,Ring,Ring
1, Ring, Ring2
phthalazine phthalazin root root
c,1|a|alpha,Ring,Ring1,n,2|b|beta,n,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,R
ing,Ring1,Ring,Ring2
phthalhydrazide root root
C,x,Ring,Ring1,(=0),x,N,x,N,x,C,x,(=0),x,c,2,Ring,Ring2,c,3,c,4,c,5,c,6,c,1,Ring
,Ring1,Ring,Ring2
fluorene fluoren root root
c,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
diphenyleneiodonium root root
[I+],9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring
3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
```

```
betacarboline root root
c,1,Ring,Ring1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,4b,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,
Ring, Ring3, n, 9 | prefhydro, c, 9a, Ring, Ring2, Ring, Ring1
carbazole carbazol root root
n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
carbazolo carbazol opfuser unknown
n,9,Ring,Ring1,c,9a,Ring,Ring2,c,1,c,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ring,Ring3,c
,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
norharman root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,n,2,c,3,c,4,c,4a,Ring,Ring2,c,5a,Ri
ng,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmane harman root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmine banisterine root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmol root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,c,3,c,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmalol root root
N, 9, Ring, Ring1, C, 9a, Ring, Ring2, C, 1, (C), x, =, x, N, 2, C, 3, C, 4, C, 4a, (, x, =, x, Ring, Ring2)
,),x,c,4b,Ring,Ring3,c,5,c,6,c,7,(0),x,c,8,c,8a,Ring,Ring3,Ring1
harmaline root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,C,3,C,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,c,7,(OC),x,c,8,c,8a,Ring,Ring3,Ring,Ring1
harmalane harmalan root root
n,9|prefhydro,Ring,Ring1,c,9a,Ring,Ring2,c,1,(C),x,n,2,C,3,C,4,c,4a,Ring,Ring2,c
,5a,Ring,Ring3,c,5,c,6,(OC),x,c,7,c,8,c,8a,Ring,Ring3,Ring,Ring1
phenanthrid root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,n,5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,9,c
,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
arsanthrid root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,[as],5,c,6,c,6a,Ring,Ring3,c,7,c,8,c,
9,c,10,c,10a,Ring,Ring3,c,10b,Ring,Ring2,Ring,Ring1
benzidine benzidin root root
N,n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2',c
,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
benzidinium root root
[N+], n, c, 4, Ring, Ring1, c, 3, c, 2, c, 1, (, x, c, 6, c, 5, Ring, Ring1,), x, c, 1', Ring, Ring2, c, 2
',c,3',c,4',(,x,[N+],n',),x,c,5',c,6',Ring,Ring2
benzidino root root
N,4@n,c,4,Ring,Ring1,c,3,c,2,c,1,(,x,c,6,c,5,Ring,Ring1,),x,c,1',Ring,Ring2,c,2'
,c,3',c,4',(,x,N,n',),x,c,5',c,6',Ring,Ring2
pyrid root root
c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
n, Ring, Ring1
pyrido|pyrid opfuser unknown
c,2|o|ortho|a|alpha,Ring,Ring1,c,3|m|meta|b|beta,c,4|p|para|g|gamma,c,5,c,6,n,1|
n, Ring, Ring1
pyridox root root
C,4,c,x,Ring,Ring1,c,x,(,x,C,5,0,x,),x,c,6,n,1,c,2,(C),x,c,3,(0),x,Ring,Ring1
pyridoxamine pyridoxamin root root
N, x, C, 4, c, x, Ring, Ring1, c, x, (,x,C,5,0,x,), x,c,6,n,1,c,2,(C), x,c,3,(O), x, Ring, Ring
```

```
pyraz root root
c,2|o|ortho,Ring,Ring1,c,3|m|meta,Ring,Ring2,.,x,n,1|n,Ring,Ring3,Ring,Ring1,.,x
n,4|p|para|n',Ring,Ring2,c,5,c,6,Ring,Ring3
pyrazino opfuser unknown
c,2|o|ortho,Ring,Ring1,c,3|m|meta,n,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyrimid root root
c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyrimido|pyrimid opfuser unknown
c,2|o|ortho,Ring,Ring1,n,3|m|meta,c,4|p|para,c,5,c,6,n,1|n,Ring,Ring1
pyridaz root root c,3,Ring,Ring1,c,4,c,5,c,6,n,1|n,n,2|n',Ring,Ring1
pyridazo|pyridazino opfuser unknown
c, 3, Ring, Ring1, c, 4, c, 5, c, 6, n, 1|n, n, 2|n', Ring, Ring1
striazine|striazin|symtriazine|symtriazin root root
c, 2, Ring, Ring1, n, 3, c, 4, n, 5, c, 6, n, 1, Ring, Ring1
astriazine astriazin asymtriazine asymtriazin root root
n, 2, Ring, Ring1, c, 3, n, 4, c, 5, c, 6, n, 1, Ring, Ring1
strioxane|strioxan|symtrioxane|symtrioxan root root
C, 2, Ring, Ring1, 0, 3, C, 4, 0, 5, C, 6, 0, 1, Ring, Ring1
astrioxane astrioxan asymtrioxane asymtrioxan root root
0,2,Ring,Ring1,C,3,0,4,C,5,C,6,0,1,Ring,Ring1
strithiane|strithian|symtrithiane|symtrithian root root
C, 2, Ring, Ring1, S, 3, C, 4, S, 5, C, 6, S, 1, Ring, Ring1
astrithiane astrithian asymtrithiane asymtrithian root root
S, 2, Ring, Ring1, C, 3, S, 4, C, 5, C, 6, S, 1, Ring, Ring1
striazino|symtriazino opfuser unknown
c, 2, Ring, Ring1, n, 3, c, 4, n, 5, c, 6, n, 1, Ring, Ring1
astriazino asymtriazino opfuser unknown
n, 2, Ring, Ring1, c, 3, n, 4, c, 5, c, 6, n, 1, Ring, Ring1
strioxano|symtrioxano opfuser unknown
C, 2, Ring, Ring1, 0, 3, C, 4, 0, 5, C, 6, 0, 1, Ring, Ring1
astrioxano asymtrioxano opfuser unknown
0,2,Ring,Ring1,C,3,0,4,C,5,C,6,0,1,Ring,Ring1
strithiano|symtrithiano opfuser unknown
C, 2, Ring, Ring1, S, 3, C, 4, S, 5, C, 6, S, 1, Ring, Ring1
astrithiano asymtrithiano opfuser unknown
S, 2, Ring, Ring1, C, 3, S, 4, C, 5, C, 6, S, 1, Ring, Ring1
borazine|borazin root root N,1,Ring,Ring1,[B],2,N,3,[B],4,N,5,[B],6,Ring,Ring1
phosphazine borazin root root n,2,Ring,Ring1,p,3,n,4,p,5,n,6,p,1,Ring,Ring1
pyrrole pyrrol root root n, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
pyrrolo pyrrol opfuser unknown n,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
pyrrolid root root N,1,Ring,Ring1,C,2|a|alpha,C,3|b|beta,C,4,C,5,Ring,Ring1
pyrrolidino root root N,4@1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
imidazole imidazol glyoxaline glyoxalin root root
c, 2, Ring, Ring1, n, 3, c, 4, =, x, c, 5, n, 1 | prefhydro, Ring, Ring1
imidazolo|imidazo|imidazo|imidaz opfuser unknown
c, 2, Ring, Ring1, n, 3, c, 4, =, x, c, 5, n, 1, Ring, Ring1
imidazolid root root C,2,Ring,Ring1,N,3,C,4,C,5,N,1,Ring,Ring1
pyrazole|pyrazol root root n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
pyrazolo|pyrazol opfuser unknown n,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
tetrazolium root root n,1,Ring,Ring1,[n+],2,n,3,n,4,c,5,Ring,Ring1
pyrazabole pyrazabol root root
c,1,Ring,Ring1,c,2,c,3,n,3a,n,8a,(,x,[B],8,),x,Ring,Ring1,.,x,[B],4,n,4a,Ring,Ri
ng2,c,5,c,6,c,7,n,7a,Ring,Ring2
isooxazole|isooxazol|isoxazole|isoxazol|isoazole|isoazol root root
o,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isooxazolo|isooxazol|isoxazolo|isoxazol opfuser unknown
o, 1, Ring, Ring1, n, 2, c, 3, c, 4, c, 5, Ring, Ring1
```

```
isooxazolid|isooxazolid|isoxazolid|isoxazolid|isoazolid|isoazolid root root
0,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
urazole urazol root root N,1,Ring,Ring1,N,2,C,3,(=0),x,N,4,C,5,(=0),x,Ring,Ring1
pyrazolid root root N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
furan|fur root root o,1,Ring,Ring1,c,2|a|alpha,c,3|b|beta,c,4,c,5,Ring,Ring1
furo opfuser unknown o,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
furfur root root C,a|alpha,c,2,Ring,Ring1,c,3,c,4,c,5,o,1,Ring,Ring1
then root root C,2,c,x,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
furazan root root c,3,Ring,Ring1,c,4,n,5,o,1,n,2,Ring,Ring1
isothiazole|isothiazol root root s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isothiazolo|isothiazol opfuser unknown s,1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isosulfonazole|isosulfonazol root root
c, 4, Ring, Ring1, c, 5, s, 1, (=, x, 0, x,) (=, x, 0, x,), x, n, 2, c, 3, Ring, Ring1
isoselenazole isoselenazol root root
[se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
isoselenazolo isoselenazol opfuser unknown
[se],1,Ring,Ring1,n,2,c,3,c,4,c,5,Ring,Ring1
benzisosulfonazole|benzisosulfonazol root root
s,1,(=,x,0,x,)(=,x,0,x,),x,Ring,Ring1,n,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
7a, Ring, Ring2, Ring, Ring1
benzsulfonazole|benzsulfonazol root root
s,1,(=,x,0,x,)(=,x,0,x,),x,Ring,Ring1,c,2,n,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,
7a, Ring, Ring2, Ring, Ring1
sulfonazole|sulfonazol root root
s, 1, (=, x, 0, x,) (=, x, 0, x,), x, Ring, Ring1, c, 2, n, 3, c, 4, c, 5, Ring, Ring1
thiophene thien root root
c, 2 a alpha, Ring, Ring1, c, 3 b beta, c, 4, c, 5, s, 1, Ring, Ring1
thieno|thien opfuser unknown c,2,Ring,Ring1,c,3,c,4,c,5,s,1,Ring,Ring1
selenophene | selenophen root root [se], 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, Ring, Ring1
selenopheno selenophen opfuser unknown
[se],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
tellurophene | tellurophen root root [Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
telluropheno tellurophen opfuser unknown
[Te],1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
piperid root root N,1|n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
piperidino root root N,401 n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,Ring,Ring1
homopiperid root root N,1 n,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
nipecot root C,a|alpha,C,3,Ring,Ring1,C,4,C,5,C,6,N,1|n,C,2,Ring,Ring1
isonipecot root root C,a|alpha,C,4,Ring,Ring1,C,5,C,6,N,1|n,C,2,C,3,Ring,Ring1
purine purin root root
n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,c,5,Ring,Ring1,R
ing,Ring2
adenine adenin root root
n, 1, Ring, Ring1, c, 2, n, 3, c, 4, (, x, c, 5, Ring, Ring2, c, 6, (, x, N, n | n6,), x, Ring, Ring1,), x,
n,9,c,8,n,7|prefhydro,Ring,Ring2
piperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4|n',C,5,C,6,Ring,Ring1
piperazino root root N,401 n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,Ring,Ring1
homopiperaz root root N,1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
homopiperazino root root N,4@1|n,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,C,7,Ring,Ring1
pyrroliz root root
n,4,Ring,Ring1,Ring,Ring2,c,5,c,6,c,7,c,7a,Ring,Ring1,c,1,c,2,c,3,Ring,Ring2
pentalene pentalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2
pentaleno pentalen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,6a,Ring,Ring1,Ring,Ring2
```

```
heptalene heptalen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,10,c,10a,Ring,R
ing1, Ring, Ring2
asindacene asindacen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,8a,
Ring, Ring3, c, 8b, Ring, Ring2, Ring, Ring1
sindacene sindacen root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,4a,Ring,Ring3,c,5,c,6,c,7,c,7a,Ring
,Ring3,c,8,c,8a,Ring,Ring2,Ring,Ring1
octalene octalen root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,6a,Ring,Ring2,c,7,c,8,c,9,c,10,c,11,c,12,c,
12a, Ring, Ring1, Ring, Ring2
mevalon root root C, 1, C, 2, C, 3, (,x,C,4,C,5,0,x,)(,x,0,x,),x,C,x
lact|lactyl root root C,1,C,2|alpha|a,(,x,0,x,),x,C,3|b|beta
24d root root
(C1,x,),x,c,5,c,6,Ring,Ring1)
245t root root
,Cl,x,),x,c,5,(,x,Cl,x,),x,c,6,Ring,Ring1
dnp | 24dnp root root c, 4@1, Ring, Ring1, c, x, ([N+] (=0) [0-
]), x, c, 3 | m | meta, c, x, ([N+] (=0) [0-]), x, c, 5, c, 6, Ring, Ring1
morphol root c,2,Ring,Ring1,C,3,N,4,C,5,C,6,O,1,Ring,Ring1
morpholino root root 0,1,Ring,Ring1,C,2,C,3,N,4@4,C,5,C,6,Ring,Ring1
semicarbazide semicarbazid root root N,1,N,2,C,x,(=,x,0,3,),x,N,4
semicarbazido root root N, 4@1, N, 2, C, x, (=, x, 0, 3,), x, N, 4
isosemicarbazide | isosemicarbazid root root N,1,N,2,C,x,(,x,0,3,)=,x,N,4
isosemicarbazido root root N, 401, N, 2, C, x, (x, 0, 3,) = x, N, 4
semicarbazono root root N, 8@1, N, 2, C, x, (=, x, 0, 3,), x, N, 4
carbaz root root C,1,N,2,N,3
acetone aceton root alkane C,1|a|alpha,C,x,(=0),x,C,3|w|omega
acetylacetone root root C,1,C,2,(=,x,0,x,),x,C,3,C,4,(=,x,0,x,),x,C,5
isobutyrone|isobutyron root root CC(C)C(=0)C(C)C,x
isovalerone|isovaleron root root CC(C)CC(=0)CC(C)C,x
enanthone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,(=0),x,C,8,
C,9,C,10,C,11,C,12,C,13|w|omega
pelargone root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(=0
),x,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega
laurone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,x,(=0),x,C,13,C,14,C,15,
C,16,C,17,C,18,C,19,C,20,C,21,C,22,C,23|w|omega
myristone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,x,(=0),x,C,15,
c,16,c,17,c,18,c,19,c,20,c,21,c,22,c,23,c,24,c,25,c,26,c,27|w|omega
palmitone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,x,(=
o),x,c,17,c,18,c,19,c,20,c,21,c,22,c,23,c,24,c,25,c,26,c,27,c,28,c,29,c,30,c,31
w omega
stearone root alkane
C,1|a|alpha,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C
,17,C,x,(=0),x,C,19,C,20,C,21,C,22,C,23,C,24,C,25,C,26,C,27,C,28,C,29,C,30,C,31,
C,32,C,33,C,34,C,35|w|omega
silatrane|silatran root root
[Si],1,Ring,Ring1,Ring,Ring2,O,2,C,3,C,4,N,5,(,x,C,6,C,7,O,8,Ring,Ring1,),x,C,11
,C,10,0,9,Ring,Ring2
```

```
glycoluril root root
N,n|1,Ring,Ring1,C,2,(=,x,0,x,),x,N,n'|3,C,3a,Ring,Ring2,N,n''|4,C,5,(=,x,0,x,),
x,N,n''' | 6,C,6a,Ring,Ring1,Ring,Ring2
acetylene acetylen root root C,1,#,x,C,2
diacetylene root root C,1, #, x,C,2,C,3, #, x,C,4
allophan root trivial C,1,(=,x,0,x,),x,N,2,C,3,(=,x,0,x,),x,N,4
biquanide|biquanid root root N, 1, C, x, (=,x,N,2,), x, N, 3, C, x, (=,x,N,4,), x, N, 5
biuret root root N,1,C,2, (=,x,0,x,),x,N,3,C,4, (=,x,0,x,),x,N,5
carbazone | carbazon root root N, 1, N, 2, C, 3, (=, x, 0, x,), x, N, 4, =, x, N, 5
carbazono root root N, 4@1, N, 2, C, 3, (=, x, 0, x, ), x, N, 4, =, x, N, 5
carbodiazone carbodiazon root root N, 1, =, x, N, 2, C, 3, (=, x, 0, x,), x, N, 4, =, x, N, 5
carbodiazono root root N, 4@1, =, x, N, 2, C, 3, (=, x, 0, x, ), x, N, 4, =, x, N, 5
carbodiimide carbodiimid root root N,n | 1, =, x,C,x,=,x,N,n' | 3
sulfurdiimide | sulfurdiimid root root N, n \mid 1, =, x, S, x, =, x, N, n' \mid 3
carbonohydrazide | carbonohydrazid | carbohydrazide | carbohydrazid | carbazid
root root N,1,N,2,C,3,(=,x,0,x,),x,N,4,N,5
carbonohydrazido | carbohydrazido | carbazido | root | root
N, 401, N, 2, C, x, (=, x, 0, x,), x, N, 4, N, 5
isocarbonohydrazide isocarbonohydrazid root root
N,1,N,2,C,x,(,x,0,x,)=,x,N,4,N,5
isocarbonohydrazido root root N, 4@1, N, 2, C, x, (,x,0,x,) = ,x,N,4,N,5
formazan root root N,1,N,2,=,x,C,3,N,4,=,x,N,5
guanidine guanidin root root N, 1 \mid n, C, x, (,x,N,3 \mid n',), x, =, x, N, 2 \mid n''
quanidino quanido root root N, 4@1, C, x, (=, x, N, 2,), x, N, 3
hydanto hydant root C,1,C,2,N,3,C,4,(=,x,0,x,),x,N,5
hydantoin root root
N, 1, Ring, Ring1, C, 2, (=, x, 0, x, ), x, N, 3, C, 4, (=, x, 0, x, ), x, C, 5, Ring, Ring1
rhodanine rhodanin root root
S,1,Ring,Ring1,C,2,(=,x,S,x,),x,N,3,C,4,(=,x,0,x,),x,C,5,Ring,Ring1
isourea|pseudourea root root N,1|n,=,x,C,x,(,x,0,2,),x,N,3|n'
lisoureido root root N, 4@1 | n, =, x, C, x, (, x, 0, 0, ), x, N, 3 | n'
3isoureido root root N, 1 | n, =, x, C, x, (,x,0,0,), x, N, 403 | n'
isothiourea root root N, 1 \mid n, =, x, C, x, (,x,S,s,), x, N, 3 \mid n'
isothiouronium root root N, 1 \mid n, =, x, C, x, (, x, [S+], s,), x, N, 3 \mid n'
lisothioureido root root N,401|n,=,x,C,x,(,x,S,s,),x,N,3|n'
3isothioureido root root N, 1 \mid n, =, x, C, x, (, x, S, s, ), x, N, 403 \mid n'
isoselenourea root root N, 1 \mid n, =, x, C, x, (,x, [Se], se,), x, N, 3 \mid n'
isoselenouronium root root N, 1 \mid n, =, x, C, x, (,x, [Se+], se,), x, N, 3 \mid n'
lisoselenoureido root root N,4@1|n,=,x,C,x,(,x,[Se],se,),x,N,3|n'
3isoselenoureido root root N, 1 \mid n, =, x, C, x, (,x, [Se], se,), x, N, 4@3 \mid n'
isotellurourea root root N, 1 | n, =, x, C, x, (, x, [Te], te,), x, N, 3 | n'
isotellurouronium root root N,1|n,=,x,C,x,(,x,[Te+],te,),x,N,3|n'
lisotelluroureido root root N,401|n,=,x,C,x,(,x,[Te],te,),x,N,3|n'
3isotelluroureido root root N,1|n,=,x,C,x,(,x,[Te],te,),x,N,403|n'
glycer pseudosugar unknown x,x
glycer root root C,1,C,2,(,x,0,a|alpha,),x,C,3,0,b|beta,
pentaerythritol root 0,x,C,x,C,x,(,x,C,x,0,x,),x,(,x,C,x,0,x,),x,C,x,0,x
pentaerythrityl root root C,40x,C,x,(,x,C,40x,),x,(,x,C,40x,),x,C,40x
alphapinene root root
C,1,Ring,Ring1,Ring2,C,2,(,x,C,10,)=,x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
betapinene root root
C,1,Ring,Ring1,Ring,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
carve|carv|carvene root root
C, 2, Ring, Ring1, C, 3, C, 4, (,x,C,8, (=,x,C,9,),x,C,10,),x,C,5,c,6,c,1, (,x,C,7,),x,Rin
g,Ring1
```

```
dihydrocarve|dihydrocarv|carvomenth root root
C, 2, Ring, Ring1, C, 3, C, 4, (,x,C,8, (=,x,C,9,),x,C,10,),x,C,5,C,6,C,1, (,x,C,7,),x,Rin
g,Ring1
carvacr root root
c, 2, Ring, Ring1, c, 3, c, 4, (,x,C,8, (,x,C,9,),x,C,10,),x,c,5,c,6,c,1, (,x,C,7,),x,Ring
betaapinene root root
C,1,Ring,Ring1,Ring2,C,2,(=,x,C,10,),x,C,3,C,4,C,5,(,x,C,6,Ring,Ring1,),x,C
,7,(,x,C,8,),x,(,x,C,9,),x,Ring,Ring2
pinacol root root
0, x, C, x, (, x, C, x,), x, (, x, C, x,), x, C, x, (, x, 0, x,), x, (, x, C, x,), x, C, x
pinacolyl root root C,40x,(,x,C,x,),x,C,x,(,x,C,x,),x,(,x,C,x,),x,C,x
pinacolone root C,1,C,2,(=,x,0,x,),x,C,3,(,x,C,x,),x,(,x,C,x,),x,C,x
benzopinacole benzopinacol root root
C,x,(,x,C,x,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,(,x,c,1',Ring,Ring1,),x,(,x,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,1',Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,4,c,5,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,c,6,Ring,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,2,Ring1,c,
Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2,),x,(0),x,),x,(,x,c,1'',Ring,Ring3,c,2
'',c,3'',c,4'',c,5'',c,6'',Ring,Ring3,),x,(,x,c,1''',Ring,Ring4,c,2''',c,3''',c,
4''',c,5''',c,6''',Ring,Ring4,),x,0,x
benzopinacolone root root
0=C(C4=CC=CC=C4)C(C2=CC=CC=C2)(C3=CC=CC=C3)C1=CC=CC=C1, x
resorcinol root root
0,0,c,1,Ring,Ring1,c,2,c,3,(,x,0,o',),x,c,4,c,5,c,6,Ring,Ring1
orsellin root root
c,2|o|ortho,Ring,Ring1,c,3,(,x,0,o',),x,c,4|p|para,c,5,(,x,0,o'',),x,c,6,c,1,(C)
,x,Ring,Ring1
olivetol root root
0,x,c,1,Ring,Ring1,c,2,c,3,(,x,0,x,),x,c,4,c,5,(CCCCC),x,c,6,Ring,Ring1
hydroquinone hydroquinon root root
c,1,Ring,Ring1,Ring,Ring2,c,2,c,3,c,4,Ring,Ring3,c,5,c,6,Ring,Ring1,.,x,0,o,Ring
,Ring2,.,x,O,o',Ring,Ring3
syring root root
C,x,c,1,Ring,Ring1,c,2,c,3,(,x,OC,x,),x,c,4,(,x,O,x,),x,c,5,(,x,OC,x,),x,c,6,Rin
g,Ring1
syringol root root
0,x,c,1,Ring,Ring1,c,2,(0C),x,c,3,c,4,c,5,c,6,(0C),x,Ring,Ring1
pyrogallol root root
0,x,c,1,Ring,Ring1,c,2,(,x,0,x,),x,c,3,(,x,0,x,),x,c,4,c,5,c,6,Ring,Ring1
orcinol root root
0,x,c,1,Ring,Ring1,c,2,c,3,(,x,0,x,),x,c,4,c,5,(,x,C,x,),x,c,6,Ring,Ring1
pyrogallitol root root
0,x,C,1,Ring,Ring1,C,2,(,x,0,x,),x,C,3,(,x,0,x,),x,C,4,C,5,C,6,Ring,Ring1
phloroglucin root root
c,1,Ring,Ring1,c,2,c,3,(,x,0,x,),x,c,4,c,5,(,x,0,x,),x,c,6,Ring,Ring1
phloroglucide root root Oc1cc(O)c(c2cc(O)cc(O)c2)c(O)c1,x
thym root root
c,3,Ring,Ring1,c,2,c,1,(,x,C,x,),x,c,6,c,5,c,4,(,x,C,x,(,x,C,x,),x,C,x,),x,Ring,
Ring1
 isopuleg root root
C,x,Ring,Ring1,C,x,C,x,(,x,C,x,),x,C,x,C,x,C,x,(,x,C,x,(=,x,C,x,),x,C,x,),x,Ring
pyrocatechol orthocatechol root root
0,x,c,1,Ring,Ring1,c,2,(,x,0,x,),x,c,3,c,4,c,5,c,6,Ring,Ring1
nitrone nitron root root C, a alpha, =, x, [N+], n, [O-], x
 glyoxime glyoxim root root C,x,(,x,C,x,=,x,N,x,0,x,),x,=,x,N,x,0,x
 coumarine coumarin cumarin root root
 o,1,Ring,Ring1,c,2,(=,x,0,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Rin
 g,Ring1,Ring,Ring2
```

```
isocoumarin isocumarin root root
g,Ring1,Ring,Ring2
coumaran root root
0,1,Ring,Ring1,C,2,C,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
coumarone coumaron root root
o,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring1,Ring,Ring
ayapin root root
o,1,Ring,Ring1,c,2,(=,x,0,x,),x,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,(,x,COC,x,Ring,R
ing3,),x,c,7,Ring,Ring3,c,8,c,8a,Ring,Ring1,Ring,Ring2
benzhvdr root root
C,a|alpha,(,x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,
c,2',c,3',c,4',c,5',c,6',Ring,Ring2
benzoguanamine benzoguanamin root root
c,1,(,x,Ring,Ring1,n,2,c,3,(,x,N,x,),x,n,4,c,5,(,x,N,x,),x,n,6,Ring,Ring1,),x,c,
1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
trit root root
C,a|alpha,Ring,Ring1,Ring,Ring2,Ring,Ring3,.,x,c,4,Ring,Ring4,Ring,Ring5,.,x,c,4
',Ring,Ring6,Ring,Ring7,.,x,c,4'',Ring,Ring8,Ring,Ring9,.,x,c,3,Ring,Ring4,c,2,c
,1,Ring,Ring1,c,6,c,5,Ring,Ring5,.,x,c,3',Ring,Ring6,c,2',c,1',Ring,Ring2,c,6',c
,5',Ring,Ring7,.,x,c,3'',Ring,Ring8,c,2'',c,1'',Ring,Ring3,c,6'',c,5'',Ring,Ring
ureth root root N,n,C,x,(=,x,0,x,),x,0,x,C,x,C,x
chalcone chalcon root root
C,a|alpha,(,x,C,x,(=,x,0,x,),x,c,1',Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Rin
g1,),x,=,x,C,b|beta,c,1,Ring,Ring2,c,2,c,3,c,4,c,5,c,6,Ring,Ring2
deoxybenzoin root root
C,a|alpha,(,x,C,x,(=0),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',
Ring, Ring2, =, x, C, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
thiurammonosulfide thiurammonosulfid root root
N, n, C, x, (=, x, S, x, ), x, S, x, C, x, (=, x, S, x, ), x, N, n'
thiuramdisulfide thiuramdisulfid root root
N, n, C, x, (=, x, S, x,), x, SS, x, C, x, (=, x, S, x,), x, N, n'
thiuramtrisulfide thiuramtrisulfid root root
N, n, C, x, (=, x, S, x,), x, SSS, x, C, x, (=, x, S, x,), x, N, n'
thiuramtetrasulfide thiuramtetrasulfid root root
N, n, C, x, (=, x, S, x,), x, SSSS, x, C, x, (=, x, S, x,), x, N, n'
mercuran root root S=C(SSC(N(C)C)=S)N(C)C,x
diacetamide diacetamid root root
N, n, (,x,C,x, (,x,=,x,0,x,),x,C,x,),x,C,x, (,x,=,x,0,x,),x,C,x
triacetamide triacetamid root root
0,x,),x,C,x
dibenzamide dibenzamid root root
x,),x,c,x,Ring,Ring2,ccccc,x,Ring,Ring2
tribenzamide tribenzamid root root
x,0,x,),x,c,x,Ring,Ring2,cccc,x,Ring,Ring2,),x,C,x,(,x,=,x,0,x,),x,c,x,Ring,Ring
q3, = x, cccc, x, Ring, Ring3
fulvene fulven root root
C, 6, =, x, C, 5, Ring, Ring1, C, 1, =, x, C, 2, C, 3, =, x, C, 4, Ring, Ring1
stilbene stilben root root
C,b|beta|a'|alpha', (=,x,C,a|alpha,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|pa
```

```
ra,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c,2'|o'|ortho',c,3'|m'|meta',c,4'|p'|p
ara',c,5',c,6',Ring,Ring2
stilbestrol|stilboestrol root root
C,b|beta,(=,x,C,a|alpha,c,1,Ring,Ring1,c,2,c,3,c,4,(0),x,c,5,c,6,Ring,Ring1,),x,
c,1',Ring,Ring2,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring2
hexestrol root root
C,b|beta,(CC)(,x,C,a|alpha,(CC),x,c,1,Ring,Ring1,c,2,c,3,c,4,(0),x,c,5,c,6,Ring,
Ring1,),x,c,1',Ring,Ring2,c,2',c,3',c,4',(0),x,c,5',c,6',Ring,Ring2
benzil root root
C(=0), x, (,x,C(=0),x,c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,),x,c,1',Ring,
Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
antipyr|antipyrene|phenazone root root
C, 4, Ring, Ring1, C, 5, (=0), x, N, 1, (,x, N, 2, (,x, C,x,), x, C, 3, (,x, C,x,), x, =, x, Ring, Ring1
,),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
glycid root root C,1,C,2|b|beta,Ring,Ring1,C,3,O,x,Ring,Ring1
ketene keten root root C=C=O,1
diketene | diketen root root C=C1CC(=0)01,x
adamant root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
noradamant root root
C,1,Ring,Ring1,Ring,Ring2,C,2,C,3,Ring,Ring3,C,4,C,5,(,x,C,6,C,7,(,x,C,8,Ring,Ri
ng1,),x,Ring,Ring3,),x,C,9,Ring,Ring2
hexamethylenetetramine hexamethylenetetramin root root
N,1,Ring,Ring1,Ring,Ring2,C,2,N,3,Ring,Ring3,C,4,N,5,(,x,C,6,N,7,(,x,C,8,Ring,Ri
ng1,),x,C,10,Ring,Ring3,),x,C,9,Ring,Ring2
pentamethylenetetramine|pentamethylenetetramin root root N12CNCN(CNC1)C2,x
fulvalene fulvalen root root
c, 2, Ring, Ring1, (,x,c,3,c,4,c,5,c,1, Ring, Ring1,) = ,x,c,2', Ring, Ring2,c,3',c,4',=,x
,c,5',c,1',Ring,Ring2
tetrathiafulvalene tetrathiafulvalen root root
C,2,Ring,Ring1,(,x,S,3,C,4,=,x,C,5,S,1,Ring,Ring1,)=,x,C,2',Ring,Ring2,S,3',C,4'
,=,x,C,5',S,1',Ring,Ring2
tetraselenafulvalene tetrathiafulvalen root root
C, 2, Ring, Ring1, (,x, [Se], 3, C, 4, =, x, C, 5, [Se], 1, Ring, Ring1,) =, x, C, 2', Ring, Ring2, [Se]
],3',C,4',=,x,C,5',[Se],1',Ring,Ring2
labd root natural
C,1,Ring,Ring1,C,2,C,3,[C@@],4,(,x,C,18,),x,(,x,C,19,),x,[C@@],5,([H]),x,Ring,Ri
ng2,C,6,C,7,[C@],8|a-r,(,x,C,17,),x,[C@@],9|a-
b, (,x,[C@],10,Ring,Ring2,Ring,Ring1,C,20,),x,C,11|a-
t,C,12,[C@],13,(,x,C,16,),x,C,14,C,15
ambros root natural C,2,Ring,Ring1,C,3,C,4,[C@@],5|a-
b, Ring, Ring2, (,x,C,15,),x,C,6|a-
r, [Ce], 7, (,x,C,11, (,x,C,12,),x,C,13,),x,C,8,C,9, [Ce],10, (,x,C,14,),x, [Cee],1 | a-
t,([H]),x,Ring,Ring2,Ring,Ring1
cedr root natural [C@@],2,Ring,Ring1,(,x,C,12,),x,C,3,C,4,[C@],5|a-
b, ([H]), x, Ring, Ring2, [C@@], 6 a-
r,(,x,C,13,),x,(,x,C,14,),x,[C@],7,(,x,C,11,Ring,Ring3,),x,[C@],8,(,x,C,15,),x,C
,9,C,10,[C@@],1|a-t,Ring,Ring1,Ring,Ring2,Ring,Ring3
cedrol root natural OC1(C)C3CC2(C(C3(C)C)CCC2C)CC1,x
apotrichothec root natural
0, 1, Ring, Ring1, [C@], 12, Ring, Ring2, (,x,C,13,),x,C,2,C,3,C,4,[C@@],5|a-
r, (x, C, 14), x, Ring, Ring2, [C@], 6 a
b, (,x,C,15,),x,Ring,Ring3,C,7,C,8,C,9,(,x,C,16,),x,C,10,[C@],11|a-
t,([H]),x,Ring,Ring3,Ring,Ring1
```

```
germacr root natural
C, 1, Ring, Ring1, C, 2, C, 3, [C0], 4, (,x,C,15,), x,C,5,C,6, [C0], 7, (,x,C,11, (,x,C,12,),x,C,12,), x,C,11, (,x,C,12,0), x,C,11, (
C, 13, ), x, C, 8, C, 9, [C@@], 10, (,x, C, 14,), x, Ring, Ring1
podocarpa podocarp root steroid
C, 1, Ring, Ring1, C, 2, C, 3, [C@e], 4, (,x,C,15|18,), x, (,x,C,16|19,), x,C,5, Ring, Ring2,C,
6,C,7,C,8,Ring,Ring3,C,14,C,13,C,12,C,11,C,9,Ring,Ring3,[C@@],10,(,x,C,17,),x,Ri
ng, Ring1, Ring, Ring2
palustr root natural
C,x,Ring,Ring4,...,x,CC(C)C(CC3)=CC2=C3[C@]1(C)C(CC2)[C@@],x,Ring,Ring4,(C)CCC1,x
gedun root natural
C,1,Ring,Ring1,C,2,C,3,C,4,(,x,C,30,),x,(,x,C,31,),x,C,5,Ring,Ring2,C,6,C,7,C,8,
Ring, Ring3, (,x,C,x,),x,C,14,Ring,Ring4,C,15,C,16,O,x,C,17,(,x,C,20,Ring,Ring5,C,
x,0,x,C,23,C,22,Ring,Ring5,),x,C,13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,R
ing3,C,10,(,x,C,19,),x,Ring,Ring2,Ring,Ring1
eudesm root natural
C,1,Ring,Ring1,C,2,C,3,[C@],4,(C),x,[C@@],5,([H]),x,Ring,Ring2,C,6,[C@],7|a-
r,(,x,C,11,(C),x,C,x,),x,C,8|a-b,C,9|a-t,[C@],10,(C),x,Ring,Ring2,Ring,Ring1
trichotheca trichothec root natural C,3,Ring,Ring1,C,4,[C@@],5|a-
r, (x, C, 14,), x, Ring, Ring2, [C@], 6 a-
b, (,x,C,15,),x,Ring,Ring3,C,7,C,8,[C@],9,(,x,C,10,[C@],11|a-
t,([H]),x,Ring,Ring3,O,1,[C@],2,Ring,Ring1,[C@],12,Ring,Ring2,C,13,),x,C,16
scirpenol root natural [C@],3,(O),x,Ring,Ring1,C,4,[C@@],5|a-
r,(,x,C,14,),x,Ring,Ring2,[C@],6|a-
b, (,x,C,15,),x,Ring,Ring3,C,7,C,8,C,9,(=,x,C,10,[C@],11,([H]),x,Ring,Ring3,O,1,[
C@], 2, Ring, Ring1, [C@@], 12, Ring, Ring2, (,x,0,x,Ring,Ring4,),x,C,13,Ring,Ring4,),x,
C, 16
prosta prost root natural C,1,C,2,C,3,C,4,C,5,C,6,C,7,[C@@H],8|a-
t, (,x,C,9,C,10,C,11,Ring,Ring1,),x,[C@H],12|a-b,Ring,Ring1,C,13|a-
r,C,14,C,15,C,16,C,17,C,18,C,19,C,20
phorbol root natural 0,x,[C@@],13,1(,x,[C@@H],12,20)[C@H]([C@@](C=C,a-
t,Ring,Ring3,CO)([H])[C@@](O)([C@@](C=C(C)C4=O)([H]),x,[C@],4|a-b,4(O)C,a-
r,3)[C@@H]2C)[C@@]1(C)C,x
tigli|tiglia root natural
C, 13, Ring, Ring1, (,x,C,12, Ring, Ring2,),x,[C@H],x,(,x,[C@@],8,(,x,C,7,=,x,C,6|a-
t,Ring,Ring3,C,20,),x,([H]),x,C,9,(,x,[C@@],10,(,x,C,1,C,2,(C),x,C,3,Ring,Ring4,
), x, ([H]), x, C, 4|a-b, Ring, Ring4, C, 5|a-b
r,Ring,Ring3,),x,[C@@H],x,Ring,Ring2,C,x,),x,[C@@],x,Ring,Ring1,(C),x,C,x
glutathionereduced root root
O=C(NCC(,x,0,1@x,)=0)C(C,x,S,s,)NC(CCC(N)C(,x,0,1@x,)=0)=0,x
glutathione root root
O=C(NCC(O)=O)[C@H](CSSC[C@H](NC(CC[C@H](N)C(O)=O)=O)C(NCC(O)=O)=O)NC(CC[C@H](N)C(O)=O)
(0) = 0) = 0, x
sphingosin|sphingosine|dihydrosphingosin|dihydrosphingosine pseudosugar unknown
X, X
sphingosin|sphingosine root root
0,x,C,1,C,2,(,x,N,n,),x,C,3,(0),x,C,4,=,x,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,1
3, C, 14, C, 15, C, 16, C, 17, C, 18
dihydrosphingosin dihydrosphingosine root root
0,x,C,1,C,2,(,x,N,x,),x,C,3,(0),x,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,
14, C, 15, C, 16, C, 17, C, 18
phenacetin root root CCOC1=CC=C(NC(C)=0)C=C1,x
xanthotoxin root root COC1=C(OC3=O)C(C=C3)=CC2=C1OC=C2,x
troxonium root root O=C(C1=CC(OC)=C(C(OC)=C1)OC)OCC[N+](CC)(CC)CC,x
triclopyr root root O,1@x,C(=0)COC(N=C(C1)C(C1)=C1)=C1C1,x
thonzonium tonzonium root root
tolonium root root NC1=CC2=C(N=C(C=C3)C(S2)=CC3=[N+](C)C)C=C1C, x
```

```
tolazoline root root C(c1ccccc1)C2=NCCN2,x
tiodonium root root ClC(C=C2)=CC=C2[I+]C1=CC=CS1,x
tiemonium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=CS3)0)CCOCC1,x
tiametonium root root CC[N+](C)(CCSCC[N+](C)(CC)C)C,x
tibezonium root root
CC[N+](CC)(C)CCSC2=NC1=C(N=C(C4=CC=C(C=C4)SC3=CC=CC=C3)C2)C=CC=C1, x
tetramisole root root C1CSC2=NC(c3ccccc3)CN12,x
suxethonium root root CC[N+](C)(CCOC(CCC(OCC[N+](C)(CC)C)=0)=0)C,x
suxamethonium succinylcholine root root
C[N+](C)(CCOC(CCC(OCC[N+](C)(C)C)=0)=0)C, X
(=0)=0, x
stilonium root root CC[N+](CC)(CCOC2=CC=C(C=C2)C=CC1=CC=CC=C1)CC,x
spiropentane root root
C,1,Ring,Ring1,C,2,C,3,Ring,Ring1,Ring,Ring2,C,4,C,5,Ring,Ring2
sorbitane | sorbitan root root O[C@@H]([C@@H]1[C@H](O)[C@@H](O)CO1)CO,x
sesamol root root OC1=CC(OCO2)=C2C=C1,x
sepazonium root root
C1C1=CC(C1)=C(COC(C4=CC=C(C=C4C1)C1)CN2C=C[N+](CCC3=CC=CC=C3)=C2)C=C1, x
scopoletin root root o1c(=0)ccc2cc(OC)c(0)cc12,x
salbutamol root CC(C)(NCC(C1=CC(C0)=C(0)C=C1)0)C, x
saccharin|glucarin|saccharine|glucarine root root C(=0)1NS(=0)(=0)c2cccc21,x
saccharide|saccharinate root root C(=0)1[N-]S(=0)(=0)c2cccc21,x
imazethapyr|pursuit root root
O=C1NC(C2=C(C(,x,0,1@x,)=0)C=C(CC)C=N2)=NC1(C)C(C)C,x
pyridoxine|pyridoxin root root CC1=NC=C(CO)C(CO)=C10,x
prolonium hydroxytriethoium root root C[N+](C)(C)CC(0)C[N+](C)(C)C, x
procaine root root Nc1ccc(C(OCCN(CC)CC)=0)cc1,x
procainamide|procaineamide root root Nc1ccc(C(NCCN(CC)CC)=0)cc1,x
pirdonium root root CC1=CC=C(C(C3=CC=CC=C3)OCC2CCCC(N+)2(C)C)C=C1,x
pentolonium|pentolinium root root C[N+]1(CCCCC[N+]2(C)CCC2)CCC1,x
lytensium|penthonium|pentamethonium root root C[N+](C)(C)CCCC[N+](C)(C)C,x
penoctonium root root O=C(OCC[N+](CC)(CC)CCCCCC)C(C2CCCC2)C1CCCC1,x
acetaminophen|paracetamol root root O=C(NC(C=C1)=CC=C10)C,X
amiben|chloramben root root 0.10x, C(=0)C1=C(C1)C(N)=CC(C1)=C1.x
chlorfenac root root 0.10x, C(=0)CC(C(C1)=CC=C1C1)=C1C1, x
actinonin root root OCC1N(C(C(C(C)C)NC(C(CC(NO)=0)CCCCC)=0)=0)CCC1,\times
aminopropylon root root O=C1N(c2cccc2)N(C)C(C)=C1NC(C(C)N(C)C)=O,x
azamethonium root root CC[N+](C)(C)CCN(C)CC[N+](C)(C)CC,x
benzathonium benzethonium root root
CC(C)(C1=CC=C(OCCOCC[N+](C)(C)CC2=CC=CC2)C=C1)CC(C)(C)C,x
methylbenzathonium methylbenzethonium root root
CC(C)(C1=CC(C)=C(OCCOCC[N+](C)(C)CC2=CC=C2)C=C1)CC(C)(C)C,x
benzilonium root root O=C(OC1C[N+](CC)(CC1)CC)C(C2=CC=CC2)(C3=CC=CC3)O, x
bevonium root root OC(C(OCC3[N+](C)(C)CCC3)=0)(C2=CC=CC=C2)C1=CC=CC=C1, x
carpronium root root COC(CCC[N+](C)(C)C)=0,x
carvone root root CC(C1=0)=CCC(C1)C(C)=C,x
cetrimonium root root CCCCCCCCCCCCC(N+)(C)(C)C,x
chloraminophen root root ClCCN(C1=CC=C(CCCC(0)=0)C=C1)CCC1,x
chloraminophenamide root root O=S(N)(C1=C(C1)C=C(N)C(S(=0)(N)=O)=C1)=O, \times O
chloramphenicol root root OC[C@@H](NC(C(Cl)Cl)=O)[C@@H](C1=CC=C([N+]([O-
]) = 0) C = C1) 0, x
chlorphonium root root CCCC[P+](CCCC)(CCCC)CC1=CC=CC=C1, x
ciclonium root root CC[N+](CC)(CCOC(C1CC2CC1C=C2)(C3=CC=CC3)C)C,x
cyclopyrronium root root CC[N+]1(CCC(OC(C(C3=CC=C3)C2CCCC2)=0)C1)C,X
cypion root root CCCC1CCCC1,x
```

```
decamethonium root root C[N+](C)(C)CCCCCCCC[N+](C)(C)C,x
deditonium root root
\texttt{CC}\left(\texttt{C1=CC=C}\left(\texttt{C=C1OCC}\left[\texttt{N+}\right]\left(\texttt{C}\right)\left(\texttt{CCCCCCCCC}\left[\texttt{N+}\right]\left(\texttt{C}\right)\left(\texttt{CCOC2=CC}\left(\texttt{C}\right)=\texttt{CC=C2C}\left(\texttt{C}\right)\texttt{C}\right)\texttt{C}\right)\texttt{C}\right)\texttt{C}\right)\texttt{C},\texttt{X}
denatonium root root CC[N+](CC(NC(C(C)=CC=C2)=C2C)=O)(CC)CC1=CC=CC=C1,x)
dicyclopentadiene root root
C,1,Ring,Ring1,c,2,c,3,C,3a,Ring,Ring2,C,4,Ring,Ring3,c,5,c,6,C,7,(,x,C,x,Ring,R
ing3,),x,C,7a,Ring,Ring2,Ring,Ring1
dimecolonium root root CC1CCCC([N+]1(C)C)C(OCC[N+](C)(C)C)=0, x
dimidium root root c1cc(N)cc2c(c3cccc3)[n+](C)c4cc(N)ccc4c21,x
dinoseb root CC(C(C=C([N+]([O-])=0)C=C1[N+]([O-])=0)=C10)CC, x
disilethylene root root [Si],1,C,2,C,3,[Si],4
disiquonium root root C[N+](CCCCCCCCC)(CCC[Si](OC)(OC)OC)CCCCCCCCC,x
dotefonium root root CN(C(C(C2=CC=CC=C2)(C3=CC=CS3)O)=O)CC[N+]1(CCCC1)C, x
ebdc root root S,1@x,C(NCCNC(,x,S,1@x,)=S)=S,x
edrophonium root root CC[N+](C)(C1=CC=CC(O)=C1)C,x
emepronium root root CC[N+](C)(C(CC(C2=CC=CC=C2)C1=CC=CC=C1)C)C, x
fentonium root root
C[N+]3(C4CCC3CC(OC(C(C5=CC=C5)CO)=O)C4)CC(C1=CC=C(C2=CC=CC=C2)C=C1)=O, x
fludazonium root root
0=C(C1=CC=C(F)C=C1)CN(C=C2)C=[N+]2CC(C4=C(C=C4)C1)C1)C1)CC3=C(C=C4)C1)C1, x
furacrin loveracid root CC1=CC(C=C2C(C(CC)=C)=O)=C(C=C2C)O1, x
fosamine | fosamin root root O=P(O)(OCC)C(N)=O,x
fubrogonium root root CC[N+](CC)(CCC(OC(C1=CC=C(O1)Br)=O)C)C,x
furtrethonium root root C[N+](C)(C)CC1=CC=CO1,x
glufosinate | glufosinat root root CP(0) (CCC(C(,x,0,1@x,)=0)N)=0,x
glycopyrronium root root OC(C1CCCC1)(C2=CC=CC=C2)C(OC(CC3)C[N+]3(C)C)=0, \times
qlyphosate|qlyphosat root root 0,10x,C(CNCP(0)(0)=0)=0,x
hexafluoronium root root
, x
hexamethonium root root C[N+](C)(CCCCC[N+](C)(C)C)C,x
hexasonium root root C[S+](CCOC(C(C2=CC=C2)C1CCCCC1)=0)C,x
hexopyrronium root root C[N+]1(CCC(OC(C(C2CCCC2)(C3=CC=C3)0)=0)C1)C,x
imazaquin root root CC(C1(N=C(C3=NC2=CC=C2C=C3C(,x,0,1@x,)=0)NC1=0)C)C,x
isoluminol root root NC1=CC=C2C(C(NNC2=0)=0)=C1,x
\label{eq:mebezonium} \mbox{mebezonium root } \mbox{Cot}(\mbox{CN+}](\mbox{C}) \mbox{ (C1CCC}(\mbox{CC2CCC}(\mbox{N+}](\mbox{C}) \mbox{ (C)}(\mbox{CC2}) \mbox{CC1})\mbox{C,} \mbox{x}
mecetronium root root CCCCCCCCCCCCC(N+)(C)(CC)C,x
chloramben root root 0.10x, C(=0)C1=C(N)C(C1)=CC(C1)=C1.x
nitronium root root O=[N+]=O,x
nifuroxime root root ON=Cc1ccc(o1)[N+](=O)[O-],x
octafonium root root CC[N+] (CCOC1=CC=C(C=C1)CC(C)(CC(C)C)C) (CC2=CC=CC2)CC, x
otilonium root root
pxydipentonium root root C[NH+](CCCCCCCCC[N+](C)(C)C)C,x
oxyphenonium root root CC[N+](CC)(CCOC(C(C1CCCCC1)(C2=CC=C2)0)=0)C, \times CC[N+](CC)(CCCCCC1)(C2=CC=C2)0)=0
oxypyrronium root root C[N+]1(CCCC1COC(C(C2CCCCC2)(C3=CC=C3)0)=0)C,x
oxysonium root root C[S+](CCOC(C(C1CCCCC1)(C2=CC=CC2)O)=O)C,x
amezinium root root COC1=CC(N)=CN=[N+]1C2=CC=CC=C2, x
amenzpyrinium root root CN(C(OC1=CC=C[N+](CC2=CC=CC=C2)=C1)=O)C,x
carcainium root root C[N+](CC(NC1=CC=CC=C1)=0)(CC(NC2=CC=CC=C2)=0)C, \times C(NC1=CC=CC=C2)=0)C
clonidine root root
\texttt{c,p,Ring,Ring1,c,m,c,x,(Cl),x,c,x,(NC2=NCCN2),x,c,x,(Cl),x,c,x,Ring,Ring1}
dequalinium root root
CC1=CC(N)=C2C(C=CC=C2)=[N+]1CCCCCCCCC(N+)(C(C)=C3)=C(C=CC=C4)C4=C3N, x
elliptinium root root CC(C2=C1C=C[N+](C)=C2)=C(C3=C4C=CC(O)=C3)C(N4)=C1C, \times C4C=C1C
```

```
fazadinium root root
CC5=C(N(C6=[N+]5C=CC=C6)N=NN3C(C2=CC=CC=C2)=C([N+]4=C3C=CC=C4)C)C1=CC=CC=C1, x=0
fenpiverinium root root C[N+]1(CCC(C2=CC=CC=C2)(C3=CC=C3)C(N)=O)CCCCC1,x
methanthelinium root root O=C(C2C3=C(C=CC=C3)OC1=CC=CC=C12)OCC[N+](CC)(C)CC,x
methylthioninium root root CN(C1=CC([S+]=C(C=C(N(C)C)C=C3)C3=N2)=C2C=C1)C, x
metocinium root root C[N+](C)(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)O)=O)C, x
nicotine root root CN1C(C2=CC=CN=C2)CCC1,x
nolinium root root ClC(C=C3)=C(Cl)C=C3NC2=CC1=CC=CC=[N+]1C=C2,x
pentolinium root root C[N+]1(CCCCC[N+]2(C)CCCC2)CCCC1,x
prifinium root root CC[N+]2(CCC(C2C)=C(C3=CC=CC=C3)C1=CC=CC=C1)CC, x
promethazine root root CC(N(C)C)CN1C3=C(C=CC=C3)SC2=C1C=CC=C2,X
pyrvinium root root
CN(C1=CC4=C([N+](C)=C(C=C4)C=CC2=C(C)N(C3=CC=CC=C3)C(C)=C2)C=C1)C, x
rosaniline rosanilin root root
N=C(C=C3)C=CC3=C(C2=CC=C(N)C(C)=C2)C1=CC=C(N)C=C1, x
senfol root root N=C=S,x
])=0)C1N=NC2=CC=C([S](=0)([O-])=0)C=C2.[Na+].[Na+].[Na+],x
thonzylaminium root root COc2cc(cc2)CN(clncccn1)CC[N+](C)C,x
trantelinium root root C[N+]1(C2CCC1CC(OC(C4C3=CC=C3OC5=C4C=CC=C5)=O)C2)C,x
trimethidinium root root CC1(C2CCC1(C[N+](CCC[N+](C)(C)C)(C2)C)C)C, x
thenium root root C[N+](CCOC2=CC=CC=C2)(C)CC1=CC=CS1,x
menrium tropium librium solium root root [0-
[N+](CC(NC)=N3)=C(C2=C3C=CC(C1)=C2)C1=CC=CC=C1, x
oxapropanium root root C[N+](C)(C)CC10C0C1,x
furium root root [O-][N+](C1=CC=C(C2=CSC(NC(C)=O)=N2)O1)=O, x
tropylium root root C1=CC=C[C+]C=C1,x
acetaminophen root root Oc1ccc(cc1)NC(=0)C,x
acetur root root CCNC(=0)C,x
afurolol root root CC(C)(NCC(COC(C=CC=C1CO2)=C1C2=O)O)C,x
agallol root root COCC[Hg]Cl,x
alizarin root root O=C(c2cccc23)c1c(O)c(O)ccc1C3=O,x
allantoin root root O=C(N1)NC(NC(N)=O)C1=O,x
amantanium root root CCCCCCCCC[N+](C)(CCOC(C23CC1CC(C3)CC(C2)C1)=0)C,x
aminopentamide root root CC(N(C)C)CC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=0,x
amprolium root root CCCC2=NC=C(C(N)=N2)C[N+]1=C(C)C=CC=C1,x
aporph root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,(C),x,C,6a,Ring,Ring3,C,7,c,7
a,Ring,Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring
2, Ring, Ring3
noraporph root root
c,1,Ring,Ring1,c,2,c,3,c,3a,Ring,Ring2,C,4,C,5,N,6,C,6a,Ring,Ring3,C,7,c,7a,Ring
Ring4,c,8,c,9,c,10,c,11,c,11a,Ring,Ring4,c,11b,Ring,Ring1,c,11c,Ring,Ring2,Ring
,Ring3
aspirin root root O=C(O)clccccclOC(C)=O,x
azaspirium root root
COC(C1=C(C(OC)=C23)C=CO1)=C3OC5=C(C[N+]4(CC5=C)CCCCC4)C2=O,X
bephenium root root C[N+](CCOC1=CC=CC=C1)(CC2=CC=CC=C2)C,x
berb root root c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,C,6,N,7|a-
r,Ring,Ring3,C,8,c,8a,Ring,Ring4,c,9,c,10,c,11,c,12,c,12a,Ring,Ring4,C,13 a-
t,C,13a|a-b,Ring,Ring3,c,13b,Ring,Ring2,Ring,Ring1
bidimazium root root
CN(C1=CC=C(C=CC2=[N+](C)C(C3=CC=C(C4=CC=CC=C4)C=C3)=CS2)C=C1)C, x
bretylium root root CC[N+](C)(CC1=C(Br)C=CC=C1)C,x
busulfan root root O=S(OCCCCOS(=O)(C)=O)(C)=O,X
carazolol root root OC(CNC(C)C)COC1=CC=CC2=C1C(C=CC=C3)=C3N2,x
clofilium root root CCCCCCC[N+](CC)(CCCCC1=CC=C(C=C1)Cl)CC,x
```

```
datelliptium root root
CC1=C4C(C=C[N+](CC[NH+](CC)CC)=C4)=C(C)C3=C1C2=C(N3)C=CC(O)=C2, x
demecarium root root
CN(C(OC2=CC=CC([N+](C)(C)C)=C2)=O)CCCCCCCCCN(C(OC1=CC=CC([N+](C)(C)C)=C1)=O)C, x
dibromantin root root CC(C(N1Br)=0)(N(Br)C1=0)C,x
diphenhydramine root root CN(C)CCOC(C2=CC=CC2)C1=CC=CC=C1,x
dithizone root root S=C(NNC2=CC=CC=C2)N=NC1=CC=CC=C1,x
dopamine root root
NCC, x, c, 1, Ring, Ring1, c, 2, c, 3, (0), x, c, 4, (0), x, c, 5, c, 6, Ring, Ring1
etipirium root root C[N+]1(CCOC(C(C2=CC=CC=C2)(C3=CC=CC=C3)0)=0)CCCC1,x
fench root root
ng1, ), x, C, 7, Ring, Ring2
feniodium root root ClC2=CC=C(C(Cl)=C2)[I+]C1=CC=C(C=C1Cl)Cl,x
flutropium root root C[N+]1(C2CCC1CC(OC(C(C3=CC=CC=C3)(C4=CC=CC=C4)O)=O)C2)CCF, x
furazolium root root [O-][N+](C1=CC=C(C2=CSC3=[N+]2CCN3)O1)=O, \times O(CC)
halopenium root root CC(C1=CC(C1)=C(C=C1)CCC(N+)(C)(CC2=CC=C(C=C2)Br)C)C)C,x
hexafluorenium root root
C[N+](C)(C2C1=C(C3=C2C=CC=C3)C=CC=C1)CCCCCC[N+](C)(C6C4=C(C5=CC=CC=C56)C=CC=C4)C
hexocyclium root root C[N+]1(CCN(CC(C2CCCCC2)(C3=CC=C3)0)CC1)C,x
ethidium | homidium root root
NC(C=C3)=CC2=C3C1=CC=C(N)C=C1C(C4=CC=CC=C4)=[N+]2CC, x
indenolol root root CC(NCC(COC2=C1C=CCC1=CC=C2)O)C,x
ionone|ionon|alphaionon|alphaionone root root O=C(C)C=CC1c(C)cCCC1(C)C,x
betaionone|betaionon root root O=C(C)C=CC1=C(C)CCCC1(C)C,x
isometamidium root root
CC[N+]4=C(C2=C(C5=CC=C(C=C45)N)C=CC(NN=NC3=CC=CC(C(N)=N)=C3)=C2)C1=CC=CC=C1,x
isophor root root C,1,Ring,Ring1,C,2,C,3,(C),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
isophorone root root
O=,x,C,1,Ring,Ring1,C,2,=,x,C,3,(C),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
lapirium root root O=C(NCCOC(CCCCCCCCC)=O)C[N+]1=CC=CC=C1,x
methylbenactyzium root root OC(C1=CC=CC=C1)(C2=CC=C2)C(OCC[N+](CC)(C)CC)=0,x
benactyzine root root CCN(CCOC(C(C1=CC=CC=C1)(C2=CC=CC=C2)0)=0)CC,x
miripirium root root CCCCCCCCCCCCC(N+)1=CC=C(C)C=C1,x
neopentylglycol root root OCC(C)(C)CO,x
nioxime root root ON=C(CCCC1)C1=NO,x
oxapium root root C[N+]1(CC2COC(C3CCCCC3)(C4=CC=CC=C4)O2)CCCCC1,x
oxolin root root CC2=CN(CC)C1=CC(OCO3)=C3C=C1C2=O,X
oxprenolol root root CC(NCC(COC1=CC=CC=C1OCC=C)O)C,x
oxybenzone root root 0=C(C1=CC=CC=C1)C(C=CC(OC)=C2)=C2O,x
penbutolol root root OC(CNC(C)(C)C)COC1=C(C2CCCC2)C=CC=C1,x
pentacynium root root
C[N+](CCCCC(C1=CC=CC=C1)(C2=CC=CC=C2)C#N)(CC[N+]3(CCOCC3)C)C,x
pentazocine root cc2c3(c)c1=cc(0)=cc=c1cc2N(cc=c(c)c)cc3,x
phenacetur root root CCNC(=0)Cclcccccl,x
phencyclidine angeldust root root c1(C2(N3CCCCC3)CCCCC2)ccccc1,x
pinaverium root root COC4=CC(Br)=C(C=C4OC)C[N+]3(CCOCC3)CCOCCC1CCC2CC1C2(C)C,x
piperylene root root C=CC=CC, x
piproctanylium root root CC(C)CCC(C)CC[N+]1(CC=C)CCCC1,x
piprocurarium root root CC[N+](CC)(CCOCCOC(C([N+]2(CCCCC2)C)C1=CC=CC=C1)=O)C,X
pranolium root root CC(C)[N+](C)(C)CC(0)COC1=C2C(C=CC=C2)=CC=C1,x
pretamazium root root
CC[N+]3=C(SC=C3C4=CC=C(C5=CC=CC=C5)C=C4)C=CC1=CC=C(N2CCCC2)C=C1, \times CCCCC2
propanolol root root OC(CNC(C)C)COC1=C2C(C=CC=C2)=CC=C1,x
```

```
propidium root root
C[N+](CC)(CC)CCC[N+](C3=C2C=CC(N)=C3)=C(C4=CC=CC=C4)C1=C2C=CC(N)=C1, \times C1, \times C2, \times C2, \times C3, \times
prospidium root root ClCC(0)CN3CC[N+]2(CC3)CC[N+]1(CC2)CCN(CC1)CC(0)CC1,x
pyritidium root root
CC1 = CC(NC2 = CC(C(C3 = CC = C(C = C3)N) = [N+](C5 = CC(N) = CC = C45)C) = C4C = C2) = NC(N) = [N+]1C, x = C2 = C45)C
quinomethionate | chinomethionate root root O=C3SC2=NC1=CC(C)=CC=C1N=C2S3,x
salicin root root O[C@H]10[C@@H](OC2=CC=CC=C2CO)[C@H](O)[C@@H](O)[C@@H]10,x
serenium root root CCOC(C=C2)=CC=C2N=NC1=CC=C(N)C=C1N,x
sintropium root root CCCC(C(OC1CC2CCC([N+]2(C(C)C)C1)=0)CCC,x
stilbazium root root
CC[N+]1=C(C=CC5=CC=C(C=C5)N4CCCC4)C=CC=C1C=CC3=CC=C(C=C3)N2CCCC2, x
timepidium root root COC2CC(C[N+](C)(C2)C)=C(C3=CC=CS3)C1=CC=CS1,x
tipetropium root root CCC[N+]1(C2CCC1CC(OC4C3=CC=C3CSC5=CC=CC=C45)C2)C,x
tiquizium root root C[N+]13CCCCC1CCC(C3)=C(C4=CC=CS4)C2=CC=CS2,x
trimethylsilyldifluoride root root [Si-](C)(C)(C)(F)F,x
tricine root root OCC(CO)(CO)NCC(O)=0,x
toliodium root root CC2=CC=C(C=C2)[I+]C1=CC=C(C=C1)C,x
trazium root root OC1(C4=CC=C(C=C4)C1)NC=N[N+]3=C1C2=CC=CC=C2C=C3,x
trepirium root root C[N+](C)(CCOC(C1CCC[N+]1(C)C)=0)C,x
tropolone tropalone root root
0 = x, c, 1, Ring, Ring1, c, 7, c, 6, c, 5, c, 4, c, 3, c, 2, Ring, Ring1, 0, x
tyloxapol root root NCCc1ccc(0)cc1,x
urocan root root
C,x,C,a|alpha,=,x,C,b|beta,c,4,Ring,Ring1,n,3,c,2,n,1|prefhydro,c,5,Ring,Ring1
verbenone root root O=C1C(C2)C(C)(C)C2C(C)=C1, x
yohimb|yohimbin loveracid root C,x,Ring,Ring6,.,x,N,1|a-
r, Ring, Ring1, C, 2, Ring, Ring2, [C0], 3, ([H]), x, Ring, Ring3, N, 4, (,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O), x, [C@H], 16, Ring, Ring6, [C@], 15, ([H]), x, Ring, Ring5, C, 14, Ring, Ring3
yohimb|yohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,C,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
yohimbine | yohimbin root root N, 1 | a-
r, Ring, Ring1, C, 2, Ring, Ring2, [C@], 3, ([H]), x, Ring, Ring3, N, 4, (,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,[C@H],17,
(O), x, [C@H], 16, (C(=0)OC), x, [C@], 15, ([H]), x, Ring, Ring5, C, 14, Ring, Ring3
oxayohimb|oxayohimba root root N,1|a-
r,Ring,Ring1,C,2,Ring,Ring2,[C@],3,([H]),x,Ring,Ring3,N,4,(,x,C,5,C,6,C,7,=,x,Ri
ng,Ring2,c,8|a-t,Ring,Ring4,c,9,c,10,c,11,c,12,c,13|a-
b,Ring,Ring4,Ring,Ring1,),x,C,21,[C@@],20,([H]),x,Ring,Ring5,C,19,C,18,O,17,C,16
,[C@],15,([H]),x,Ring,Ring5,C,14,Ring,Ring3
morphinan root natural c,1,Ring,Ring1,c,2,c,3,c,4,c,12|a-t,Ring,Ring2,[C@],13|a-
b,Ring,Ring4,Ring,Ring3,C,5,C,6,C,7,C,8,[C@@],14,Ring,Ring3,([H]),x,[C@],9|a-
r, (,x,N,17,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
morphine root natural
c,1,Ring,Ring1,c,2,c,3,(0),x,c,4,(,x,0,x,Ring,Ring5,),x,c,12|a-
t, Ring, Ring2, [C@], 13 a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,R
ing3, ([H]), x, [C@], 9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
codeine root natural
c, 1, Ring, Ring1, c, 2, c, 3, (OC), x, c, 4, (, x, 0, x, Ring, Ring5,), x, c, 12 | a-
t, Ring, Ring2, [C@], 13 a-
```

```
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,[C@@],6,(O),x,C,7,=,x,C,8,[C@@],14,Ring,R
ing3,([H]),x,[C@],9|a-
r, (,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
codeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,0,x,Ring,Ring5,),x,c,12|a-
t, Ring, Ring2, [C@], 13 | a-
b, Ring, Ring4, Ring, Ring3, C, 5, Ring, Ring5, C, 6, (=0), x, C, 7, =, x, C, 8, [C@@], 14, Ring, Ring
3,([H]),x,[C@],9|a-
r.(.x.N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
dihydrocodeinone hydrocodeinone root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,0,x,Ring,Ring5,),x,c,12|a-
t, Ring, Ring2, [C@], 13 a-
b, Ring, Ring4, Ring4, Ring3, C, 5, Ring, Ring5, C, 6, (=0), x, C, 7, =, x, C, 8, [C@@], 14, Ring, Ring
3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
thebacon root natural
c,1,Ring,Ring1,c,2,c,3,(OC),x,c,4,(,x,0,x,Ring,Ring5,),x,c,12|a-
t, Ring, Ring2, [C@], 13 a-
b,Ring,Ring4,Ring,Ring3,C,5,Ring,Ring5,C,6,(OC(=O)C),x,=,x,C,7,C,8,[C@@],14,Ring
,Ring3,([H]),x,[C@],9|a-
r,(,x,N,17,(C),x,C,16,C,15,Ring,Ring4,),x,C,10,c,11,Ring,Ring2,Ring,Ring1
ergoline ergolin root natural
n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Ring3,N,6,C,7,C,8|a-
t,C,9|a-b,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lyserg root natural
C,x,Ring,Ring5,.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H]),x,Ring,Rin
g3,N,6,(C),x,C,7,[C@],8|a-t,Ring,Ring5,C,9|a-b,=,x,C,10|a-
r,Ring,Ring3,c,11,Ring,Ring4,c,12,c,13,c,14,c,15,Ring,Ring1,c,16,Ring,Ring2,Ring
,Ring4
lysergide root natural
C,x,Ring,Ring5,(=0)N(CC)CC.,x,n,1,Ring,Ring1,c,2,c,3,Ring,Ring2,C,4,[C@],5,([H])
x, Ring, Ring3, N, 6, (C), x, C, 7, [C@], 8|a-t, Ring, Ring5, C, 9|a-b, =, x, C, 10|a-b, 
r, Ring, Ring3, c, 11, Ring, Ring4, c, 12, c, 13, c, 14, c, 15, Ring, Ring1, c, 16, Ring, Ring2, Ring
,Ring4
ergotaman root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1, Ring, Ring3, c, x, c, x, c, x, c, x, (, x, N, 1, c, 2, Ring, Ring4,), x, c, x, Ring, Ring3, c, x, Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,N,x,[
C@], 2', Ring, Ring5, C, 3', N, 4', Ring, Ring6, C, 5', C, 6', N, 7', Ring, Ring7, C, 8', C, 9', C, 10'
,[C@],11',([H]),x,Ring,Ring7,[C@@H],12',Ring,Ring6,0,1',Ring,Ring5
ergocornine ergocornin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
,x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
,12',(0),x,Ring,Ring6,O,1',Ring,Ring5
ergocorninine ergocorninin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
1,12',(0),x,Ring,Ring6,0,1',Ring,Ring5
ergocristine ergocristin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(Cc9ccc
```

```
cc9),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[
C@@],12',(0),x,Ring,Ring6,0,1',Ring,Ring5
ergocryptine|ergocryptin|ergocriptine|ergocriptin|alphaergocryptine|alphaergocry
ptin|alphaergocriptine|alphaergocriptin root natural c,a-t,Ring,Ring1,c,a-
b, Ring, Ring2, c, a-
1, Ring, Ring3, c, x, c, x, c, x, c, x, (x, N, 1, c, 2, Ring, Ring4,), x, c, x, Ring, Ring3, c, x, Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C
),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(0),x,Ring,Ring6,0,1',Ring,Ring5
betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
bergocryptin|bergocriptine|bergocriptin root natural c,a-t,Ring,Ring1,c,a-
b, Ring, Ring2, c, a-
1, Ring, Ring3, c, x, c, x, c, x, c, x, (,x,N,1,c,2,Ring,Ring4,), x, c, x, Ring, Ring3, c, x, Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0),
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(C(C)CC
),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@
],12',(0),x,Ring,Ring6,0,1',Ring,Ring5
ergocryptinine|ergocryptinin|ergocriptinine|ergocriptinin|alphaergocryptinine|al
phaergocryptinin alphaergocriptinine alphaergocriptinin root natural c,a-
t, Ring, Ring1, c, a-b, Ring, Ring2, c, a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0)
x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)
C),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@
@],12',(0),x,Ring,Ring6,O,1',Ring,Ring5
betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
ryptinine|bergocryptinin|bergocriptinine|bergocriptinin root natural c,a-
t, Ring, Ring1, c, a-b, Ring, Ring2, c, a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0)
,x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C)
C),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@
@],12',(0),x,Ring,Ring6,O,1',Ring,Ring5
ergosine|ergosin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1, Ring, Ring3, c, x, c, x, c, x, c, x, (x, N, 1, c, 2, Ring, Ring4,), x, c, x, Ring, Ring3, c, x, Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0),
x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,
C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12
', (0), x, Ring, Ring6, 0, 1', Ring, Ring5
ergotamine|ergotamin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
1,Ring,Ring3,c,x,c,x,c,x,c,x,(,x,N,1,c,2,Ring,Ring4,),x,c,x,Ring,Ring3,c,x,Ring,
Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=0),
x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',(Cc9cccc9)
,x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@]
,12',(0),x,Ring,Ring6,O,1',Ring,Ring5
bromocryptine|bromocryptin|bromocriptine|bromocriptin root natural c,a-
t, Ring, Ring1, c, a-b, Ring, Ring2, c, a-
1, Ring, Ring3, c, x, c, x, c, x, c, x, (x, x, 1, c, 2, (Br), x, Ring, Ring4,), x, c, x, Ring, Ring3, c,
x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,1
8, (=0),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=0),x,N,4',Ring,Ring6,[C@@H],5',
(CC(C)C),x,C,6',(=0),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Rin
g7, [C@@], 12', (0), x, Ring, Ring6, 0, 1', Ring, Ring5
ecgonidine ecgonidin root root
[C@@], x, ([H]), x, Ring, Ring1, Ring2, C, x, c, x, c, x, (, x, C, x, (=0), x, 0, 1@x,), x, [C@],
x, ([H]), x, (,x,N,x, (C), x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2
```

```
ecgonine ecgonin root root
[C@@], x, ([H]), x, Ring, Ring1, Ring2, C, x, [C@H], x, (0), x, [C@H], x, (,x,C,x, (=0), x, 0)
,1@x,),x,[C@],x,([H]),x,(,x,N,x,(C),x,Ring,Ring1,),x,C,x,C,x,Ring,Ring2
methylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(C),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,c
,2',c,3',[n+],4',(C),x,c,5',c,6',Ring,Ring2
ethylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(CC),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring,Ring2,
c,2',c,3',[n+],4',(CC),x,c,5',c,6',Ring,Ring2
benzylviologen root root
c,1,Ring,Ring1,(,x,c,2,c,3,[n+],4,(Cc3ccccc3),x,c,5,c,6,Ring,Ring1,),x,c,1',Ring
,Ring2,c,2',c,3',[n+],4',(Cc4cccc4),x,c,5',c,6',Ring,Ring2
pheneturide root root O=C(N)NC(C(CC)C1=CC=CC=C1)=O, x
lactide | dilactide root root CC(OC1=0)C(OC1C)=0,x
gallion root root OC(C(Cl)=CC([N+]([O-
])=0)=C3)=C3N=NC1=C(S(=0)(0)=0)C=C(C=C(S(=0)(0)=0)C=C2N)C2=C10,\times
clofibr root root CC(C)(OC1=CC=C(C=C1)Cl)C,x
paraben root root 0,10x,C(C1=CC=C(0)C=C1)=0,x
edetate|versenate|edta root root
0.10x, C(CN(CC(,x,0,10x,)=0)CCN(CC(,x,0,10x,)=0)CC(,x,0,10x,)=0)=0,x
fusar root root CC1=CC=C(CCCC)C=N1,x
lironion root root COC1=CC=C(OC2=CC=C(C=C2)NC(N(C)C)=O)C=C1, x
thionalide root root O=C(CS)NC2=CC1=CC=CC=C1C=C2,x
tolperisone root root CC(C(C2=CC=C(C)C=C2)=0)CN1CCCCC1,x
valethamate root root CCC(C(C(CC(N+)(CC)C)=0)C1=CC=CC=C1)C, x
secbutabarbital|butalan root root O=C(N1)NC(C(C(C)CC)(CC)C1=0)=0,x
furalan root root O=C(N2)N(CC2=0)N=CC1=CC=C([N+]([O-])=0)O1,x
boc | tboc root nprotect C,4@x,(=0)OC(C)(C)C,x
z-nprot root nprotect C,4@x,(=0)OCclcccccl,x
msoc root nprotect C,40x, (=0)OCCS(=0)(=0)C,x
cbz root nprotect
C,40x,(=0)OC,x,C,1,Ring,Ring1,=,x,C,2,C,3,=,x,C,4,C,5,=,x,C,6,Ring,Ring1
fmoc root nprotect C,40x,(=0)OCC1C2=CC=CC=C(C3=CC=CC3)2,x
dansyl root nprotect S,40x,(C2=CC=CC1=C(N(C)C)C=CC=C12)(=0)=0,x
dabsyl root nprotect S,40x,(c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(=0)=0,x
bansyl root nprotect S,40x, (C2=CC=CC1=C(N(CCCC)CCCC)C=CC=C12)(=0)=0, x
nps root nprotect S,40x,c1c([N+](=0)[0-])cccc1,x
tfa root nprotect C,40x,(=0)C(F)(F)F,x
acm root nprotect C, 4@x, NC(=0)C, x
phacm root nprotect C, 40x, NC (=0) Cc1ccccc1, x
creatine root root CN(C(N)=N)CC(O)=O,x
panthenol root root CC(CO)(C(C(NCCCO)=O)O)C,x
alanate root root [AlH4-],x
cyanamide root root NC#N,x
eprolin root root CC1=C2C(OC(CCCC(C)CCCC(C)CCCC(C)C)(C)CC2)=C(C)C(C)=C10,x
eserine|physostigmine root root O=C(NC)OC1=CC=C(N(C)C3C2(C)CCN3C)C2=C1,x
prolan root root CC([N+]([O-])=0)C(C2=CC=C(C1)C=C2)C1=CC=C(C1)C=C1,x
tropanserin root root CN1C2CCC1CC(OC(C3=CC(C)=CC(C)=C3)=O)C2,x
butanserin root root FC1=CC=C(C(C4CCN(CC4)CCCCN3C(NC2=CC=C2C3=0)=0)=0)C=C1,x
amiprol|domalium|kiatrium|levium|relanium|tensium|umbrium|velium|valium root
root O=C1CN=C(C3=CC=CC=C3)C2=C(C=CC(C1)=C2)N1C, x
prolate root root S=P(OC)(OC)SCN1C(C(C=CC=C2)=C2C1=0)=0, x
adaprolol root root CC(NCC(COC4=CC=C(C=C4)CC(OCCC23CC1CC(C3)CC(C2)C1)=0)0)C,x
agmatine root root NC(NCCCCN)=N, x
algolysin root root CCC(C(C1=CC=CC=C1)(C2=CC=CC=C2)CC(C)N(C)C)=0.[H]C1, x
altanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=C3C4=0)=S)CC2)=0)C=C1,x
```

```
angelicin root root
c,1,Ring,Ring1,c,2,o,3,c,3a,Ring,Ring2,c,4,c,5,c,5a,Ring,Ring3,c,6,c,7,c,8,(=0),
x, o, 9, c, 9a, Ring, Ring3, c, 9b, Ring, Ring2, Ring, Ring1
asparagusate root root OC(C1CSSC1)=0,x
aspartame root root O=C(OC)C(NC(C(N)CC(O)=O)=O)CC1=CC=CC=C1, x
bisoprolol root root OC(CNC(C)C)COC1=CC=C(COCCOC(C)C)C=C1,x
bornaprolol root root OC(CN(CC)C)CC1=CC=CC=C1C2C3CCC(C3)C2,x
broncholysin root root OC(C(CS)NC(C)=0)=0, x
bunaprolast root root CCCCC2=C(OC(C)=0)C1=CC=CC=C1C(OC)=C2,x
butethal root root CCCCC(C(NC1=0)=0)(C(N1)=0)CC,x
capsaicin root root O=C(CCCC/C=C/C(C)C)NCc1ccc(O)c(OC)c1,x
carbachol root root C[N+](C)(C)CCOC(N)=0,x
carlsoprol root CC(COC(N)=0)(CCC)COC(NC(C)C)=0, x
caryolysine root root ClCCN(C)CCCl,x
chloral root root O=CC(Cl)(Cl)Cl,x
chloralhydrate root root OC(0)C(Cl)(Cl)Cl,x
bromal root root O=CC(Br)(Br)Br,x
bromalhydrate root root OC(O)C(Br)(Br)Br,x
chrysanthemum | chrysanthem root root C1C(C=C(C)C)C(C)(C)1,x
cinanserin root root CN(CCCSC1=CC=CC=C1NC(C=CC2=CC=CC2)=O)C,x
clemeprol root CN(CC(C(C2=CC=CC(C1)=C2)C1=CC=CC=C1)O)C,x
coumal root root Cc1ccc(=0)oc1,x
creatinine root root N1C(=N)N(C)CC(=O)1,x
cyclen root root
N,1,Ring,Ring1,C,2,C,3,N,4,C,5,C,6,N,7,C,8,C,9,N,10,C,11,C,12,Ring,Ring1
cyprolidol root root OC(C3=CC=CC=C3)(C4=CC=CC=C4)C1CC1C2=CC=NC=C2,x
deprol root CC(COC(N)=0)(CCC)COC(N)=0, x
dibuprol root root CCCCOCC(0)COCCCC, x
eburnamonine root root O=C2N(c3ccccc34)C1=C4CCN5C1C(CCC5)(CC)C2,x
exaprolol root root CC(NCC(COC1=CC=CC=C1C2CCCCC2)0)C,x
epichlorohydrin root root ClCC1CO1,x
epithiochlorohydrin root root ClCC1CS1,x
epifluorohydrin root root FCC1CO1,x
epibromohydrin root root BrCC1CO1,x
erban root root O=C(CC)NC1=CC(Cl)=C(Cl)C=C1,x
ethacryn root root CCOC1=C(C1)C(C1)=C(C=C1)C(C(CC)=C)=0, x
farmiserina|cycloserine|cycloserin|micoserina root root NC(CON1)C1=0,x
fascaplysin root root O=C(C5=C4C=CC=C5)C1=[N+]4C=CC2=C1NC3=C2C=CC=C3, x
febuprol root root CCCCOCC(0)COC1=CC=CC=C1, x
fermine root root O=C(OC)C1=CC=CC=C1C(OC)=O,x
fertilysin root root O=C(C(Cl)Cl)NCCCCCCCCCC(C(Cl)Cl)=O,x
formamidinedisulfide root root NC(SSC(N)=N)=N,x
ftorafur root root O=C(N1)N(C2CCCO2)C=C(F)C1=O,x
geneserine|eseridine root root CC23C1=CC(OC(NC)=0)=CC=C1N(C)C2ON(CC3)C,x
glutim pidol root root C,x,C,5,Ring,Ring1,C,4,C,3,C,2,(=0),x,N,1,Ring,Ring1
hexethal root root O=C(N1)NC(C(CCCCCC)(CC)C1=0)=O,x
ibuprofen root root C(C)(C)Cclccc(ccl)C(C)C(=0)0,x
indameth root root ClC(C=C3)=CC=C3C(N2C(C)=C(CC(O)=O)C1=CC(OC)=CC=C12)=O, x
iridocin root root NC(C1=CC(CC)=NC=C1)=S,x
isatoicanhydride root root
O=C(O2)c,1,Ring,Ring1,c,6,c,5,c,4,c,3,c,2,Ring,Ring1,NC2=0,x
isoprene root root C=CC(=C)C,x
isoxaprolol root root CC1=NOC(C=CC2=CC=CC2CC(CNC(C)(C)(C)(O))=C1.x
ketanserin root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=C3C4=0)=0)CC2)=0)C=C1,x
```

```
limonene root root
C,7,c,1,Ring,Ring1,c,2,C,3,C,4,(,x,C,8,(=,x,C,9,),x,C,10,),x,C,5,C,6,Ring,Ring1
meprol | meproleaf root root CC(COC(N)=0)(CCC)COC(N)=0, x
metoprolol root root COCCC1=CC=C(OCC(O)CNC(C)C)C=C1,x
mianserin root root CN1CCN3C(C2=C(CC4=CC=CC=C34)C=CC=C2)C1,x
moprolol root root COC(C=CC=C1)=C1OCC(CNC(C)C)O,x
myrtan root root CC1CCC(C2)C(C)(C)C21,x
myrten root root CC1=CCC(C2)C(C)(C)C21,x
nicainoprol root root CC(NCC(COC1=CC=CC2=C1N(C(C3=CC=CN=C3)=O)CCC2)O)C,x
nitrogendioxide root root 0,x,=,x,[N+],16@x,[O-],x
nitricoxide root root N,32@x,=0,x
nitrousoxide root root N#[N+][O-],x
ozone|trioxygen root root O=[O+][O-],x
oxaceprol root root CC(N1CC(CC1C(0)=0)0)=0,x
pelanserin root root O=C2NC1=CC=CC=C1C(N2CCCN3CCN(C4=CC=CC=C4)CC3)=O,x
phencyclone root root O=c(c(c5c3c4ccccc4c6cccc56)c2ccccc2)c3c1ccccc1,x
phenindione root root O=C(C2=C1C=CC=C2)C(C3=CC=CC=C3)C1=O,x
propranolol root root OC(CNC(C)C)COclcccc2cccc12,x
psoralen root root
o,1,Ring,Ring1,c,2,(=0),x,c,3,c,4,c,x,Ring,Ring2,c,5,c,x,Ring,Ring3,c,4',c,5',o,
x,c,x,Ring,Ring3,c,8|8',c,x,Ring,Ring2,Ring,Ring1
thioct root root CCCCCC1SSCC1,x
phosphoramide | phosphorustriamide root root P(=0),x,(,x,N,n,)(,x,N,n',),x,N,n''
pyrophosphoramide diphosphoramide root root
P(=0),x,(,x,N,n,)(,x,N,n',),x,O,x,P(=0),x,(,x,N,n'',),x,N,n'''
prolintane root root CCCC(N2CCCC2)CC1=CC=CC=C1,x
resorufin root root
c,7,Ring,Ring1,c,6,c,5a,Ring,Ring2,o,5,c,4a,Ring,Ring3,c,4,c,3,(=0),x,c,2,c,1,c,
10a, Ring, Ring3, n, 10, c, 9a, Ring, Ring2, c, 9, c, 8, Ring, Ring1
retin root root
C, 15, C, 14, =, x, C, 13, (,x, C, 20,), x, C, 12, =, x, C, 11, C, 10, =, x, C, 9, (,x, C, 19,), x, C, 8, =, x, C, 11, C, 10, =, x, C, 11, C, 11,
C,7,C,6,Ring,Ring1,=,x,C,5,(,x,C,18,),x,C,4,C,3,C,2,C,1,(,x,C,16,)(,x,C,17,),x,R
ing, Ring1
ritanserin root root
CC(N=C1SC=CN12) = C(CCN3CCC(CC3) = C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O, x
seganserin root root
CC(NC1=CC=CC=[N]12)=C(CCN3CCC(CC3)=C(C5=CC=C(C=C5)F)C4=CC=C(C=C4)F)C2=O, x
vinylsulfurol root root C=CC1=C(C)N=CS1,x
teoprolol root root
CC(NCC(COC3=CC=CC4=C3C=C(C)N4)O)CCN1C=NC(N(C(N2C)=O)C)=C1C2=O, x
terbuprol root root COCC(COC(C)(C)C)O,x
thyropropion aminoacid ine
C,x,C,a|alpha,C,b|beta,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,0,x,C
1', Ring, Ring3, =, x, C, 2', C, 3', =, x, C, 4', (,x,0,x,),x,C,5', =,x,C,6', Ring, Ring3,),x,C
,5,=,x,C,6,Ring,Ring2
thyroacet aminoacid ine
C,x,C,a|alpha,C,1,Ring,Ring2,=,x,C,2|ortho,C,3|m|meta,=,x,C,4,(,x,0,x,C,1',Ring,
Ring3,=,x,C,2',C,3',=,x,C,4',(,x,O,x,),x,C,5',=,x,C,6',Ring,Ring3,),x,C,5,=,x,C,
6, Ring, Ring2
toliprolol root root CC(NCC(COC1=CC=CC(C)=C1)0)C,x
tolysin root root O=C(C1=C3C(C=CC(C)=C3)=NC(C2=CC=C2)=C1)OCC, x
tomoxiprole root root COC1=CC=C(C4=NC2=C(N4C(C)C)C=CC3=CC=CC=C23)C=C1,x
tricyclene tricyclen root root CC12C(C2C3)CC3C1(C)C,x
triprolidine root root CC1=CC=C(C(C3=NC=CC=C3)=CCN2CCCC2)C=C1,x
tranexam root root C[C@H]1CC[C@H](CN)CC1,x
tropicamide root root OCC(C(N(CC)CC2=CC=NC=C2)=O)C1=CC=CC=C1,x
zipeprol root root COC(C3=CC=CC=C3)CN1CCN(CC(C(C2=CC=CC=C2)OC)O)CC1,x
```

```
thioindigo root root O=C1C4=C(C=CC=C4)SC1=C2SC(C=CC=C3)=C3C2=O, x
theophyllol root root O=C1C2=C(NC=N2)N(C)C(N1C)=O.O=C([O-])C.[Na+], \times COOLORD = COOL
synephrine root root OC1=CC=C(C(O)CNC)C=C1,x
sulfathiazole root root NC1=CC=C(S(NC2=NC=CS2)(=0)=0)C=C1,x
sulfadiazine root root
0=S(N,x,c,2,Ring,Ring1,n,3,c,4,c,5,c,6,n,1,Ring,Ring1,)(C2=CC=C(N)C=C2)=O,x
strychnine root root O=C(C5)N(C4C2(CC7)C(N7C6)CC3C6=CCOC5C34)C1=C2C=CC=C1,x
squalane root root CC(CCCCC(C)CCCC(C)CCCC(C)C)CCCC(C)CCCC(C)C,x
squalene root root CC(C)=CCC(C(C)=CCCC(C)=CCCC(C)CCC=C(C)CCC=C(C)C)/C,x
spermine neuridine musculamine gerontine root root NCCCNCCCCNCCCN,x
spermidine root root NCCCNCCCCN, x
scopolamine root root CN1C2CC(OC(C(CO)c4ccccc4)=0)CC1C3C2O3,x
genoscopolamine root root C[N+]([O-])1C2CC(OC(C(CO)C4=CC=CC+C4)=O)CC1C3C2O3, x
sendachromeal root root O=C(C(C(0)=0)=C2)C=CC2=C(C)C1=CC(C(0)=0)=C(0)C=C1, x
sorb root root C,1,C,2,=,x,C,3,C,4,=,x,C,5,C,6
quercitin root root OC1=CC(C(O3)=C(O)C(C2=C3C=C(O)C=C2O)=O)=CC=C1O, x
pulegone root root CC1CC(=0)C(=C(C)C)CC1,x
benzindopyrine|benzindopyrin root root c(CCc2ccncc2)(cn3Cc4ccccc4)c1c3cccc1,x
benziodarone|benziodaron root root O=C(c3cc(I)c(O)c(I)c3)c2c1ccccc1oc2CC,x
benzopyrronium root root C[N+]1(CCC(OC(C(c2cccc2)(c3ccccc3)O)=O)C1)C,x
benzothiozane|benzothiozan root root O=C(C)Nc1ccc(C=NNC(N)=S)cc1,x
benzpiperylone|benzpiperylon root root
O=C1C(Cc3ccccc3)=C(c4ccccc4)NN1C2CCN(C)CC2, x
benzpyrinium root root CN(C(Oclc[n+](Cc2cccc2)ccc1)=0)C,x
benzquinamide benzquinamid root root
CCN(C(C3CN2CCc1c(C2CC3OC(C)=0)cc(OC)c(OC)c1)=0)CC, x
benzthiazide benzthiazid root root
0=S2(c1cc(S(N)(=0)=0)c(C1)cc1N=C(CSCc3ccccc3)N2)=0,x
benzthiazuron root root O=C(NC)Nc2sc1ccccc1n2,x
methabenzthiazuron root root O=C(NC)N(C)c2sc1ccccc1n2,x
benzvalene|benzvalen root root C13C=CC2C1C23,x
abscis absciss root root
C, 1, C, 2, =, x, C, 3, (C), x, C, 4, =, x, C, 5, C, 6, (C(C)(C1)C)(C(C)=CC1=O)O, x
mobenzoxamine mobenzoxamin root root
COclccc(C(c4cccc4)OCCN3CCN(CC3)CCC(c2ccc(F)cc2)=0)cc1,x
quinuclidine quinuclidin root root
N, 1, Ring, Ring1, Ring2, C, 2, C, 3, C, 4, (,x, C, 5, C, 6, Ring, Ring1,), x, C, 7, C, 8, Ring, Ri
ng2
uranine root root O=C3C=CC2=C(C4=CC=CC=C4C([O-])=O)C1=CC=C([O-
) C=C1CC2=C3.[Na+].[Na+], x
(=0)=0)C=C2)C=C1S([O-])(=0)=0.[Na+].[Na+],x
 furaneol root root CC10C(C)=C(0)C1=0,x
bicine|bicin root root O=C(O)CN(CCO)CCO,x
 indanthrone root root
O=C(C3=C2C=CC=C3)C1=C(NC4=CC=C(C6=0)C(C(C7=CC=CC=C67)=0)=C4N5)C5=CC=C1C2=0,×
methone dimedone root root
C,1,(=0),x,Ring,Ring1,C,2,C,3,(=0),x,C,4,C,5,(C)(C),x,C,6,Ring,Ring1
acrinol root NC1=C(C=C(OCC)C=C3)C3=NC2=C1C=CC(N)=C2.CC(O)C(O)=O, x
danthron root root 0=C(C2=C1C=CC=C20)C(C(0)=CC=C3)=C3C1=0,x
caffeine caffein root O=C(N(C)C2=C1N(C)C=N2)N(C)C1=O,x
betahistine root root CNCCclnccccl, x
pyranine root root [0-]S(C(C=C40)=C1C=CC2=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)=0)C=C(S([0-])(=0)C(S([0-])(=0)=0)C=C(S([0-])(=0)C(S([0-])(=0)=0)C=C(S([0-])(=0)C(S([0-])(=0)=0)C=C(S([0-])(=0)C(S([0-])(=0)=0)C=C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])(=0)C(S([0-])
 ]) (=0)=0) C3=CC=C4C1=C23) (=0)=0. [Na+]. [Na+]. [Na+], x
 abiet root root C,x,[C@],a-
 r, 2(C)C1[C00]([C00](CCc(C(C)C)c3)([H])C3=CC1)(C,x,C,a-t,C,a-b,2)C,x
```

```
betulin loveracid root
     C[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@@H](O)CC[C@]1(C)[C@@]2([H])CCC
     3[C@@]4([H])[C@H](C(C)=C)CC5,x
     betulin root root
     OC[C@@]45CC[C@@]3(C)[C@]2(C)CC[C@@]1([H])C(C)(C)[C@@H](O)CC[C@]1(C)[C@@]2([H])CC
     C3[C@@]4([H])[C@H](C(C)=C)CC5, x
     caluros root root CC(C)(c1ccccc1)CC=C(C)C,x
     thymine|thymin|uracil|orot|isoorot|cytosine|isocytosine|guanine|xanthine|hypoxan
     thine pseudosugar unknown x,x
     thymine thymin root root
     N, 1, Ring, Ring1, C, 2, (=0), x, N, 3, C, 4, (=0), x, c, 5, (C), x, c, 6, Ring, Ring1
     uracil root root N,1,Ring,Ring1,C,2,(=0),x,N,3,C,4,(=0),x,c,5,c,6,Ring,Ring1
     orot root C,x,c,6,Ring,Ring1,N,1,C,2,(=0),x,N,3,C,4,(=0),x,c,5,Ring,Ring1
     isoorot root root
     C, x, c, 5, Ring, Ring1, c, 6, n, 1, c, 2, (=0), x, n, 3, c, 4, (=0), x, Ring, Ring1
     cytosine root root
     n,1|prefhydro,Ring,Ring1,c,2,(=0),x,n,3,c,4,(N),n,c,5,c,6,Ring,Ring1
     isocytosine root root
     n,1|prefhydro,Ring,Ring1,c,2,(N),x,n,3,c,4,(=0),n,c,5,c,6,Ring,Ring1
     guanine pseudosugar unknown x,x
     guanine root root
     n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(N),n,N,1,c,6,(=0),x,c,5
     ,Ring,Ring1,Ring,Ring2
     xanthine root root
j
     n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,(=0),x,n,1,c,6,(=0),x,c,
5, Ring, Ring1, Ring, Ring2
hypoxanthine root root
ľ.
     n,7|prefhydro,Ring,Ring1,c,8,n,9,c,4,Ring,Ring2,n,3,c,2,n,1,c,6,(0),x,c,5,Ring,R
     ing1, Ring, Ring2
Ü
     theophylline theophyllin aminophylline aminophyllin root root
.....
     n, 7, Ring, Ring1, c, 8, n, 9, c, 4, Ring, Ring2, n, 3, (C), x, c, 2, (=0), x, n, 1, (C), x, c, 6, (=0), x,
     c,5,Ring,Ring1,Ring,Ring2
     theobromine theobromin root root
1
     n,7,Ring,Ring1,(C),x,c,8,n,9,c,4,Ring,Ring2,n,3,(C),x,c,2,(=0),x,n,1,c,6,(=0),x,
ľ
     c,5,Ring,Ring1,Ring,Ring2
ı.L
     xanthopterin root root Oc1nc(N)nc2c1nc(O)cn2,x
.4
     isoxanthopterin root root O=C1C(N=CC2=O)=C(N2)NC(N)=N1,x
xanthopterid root root
     n, 1, Ring, Ring 1, c, 2, (N), x, n, 3, c, 4, (O), x, c, 4a, Ring, Ring 2, n, 5, c, 6, (O), x, c, 7, n, 8, c, 8
a, Ring, Ring1, Ring, Ring2
     pterin|pterine root root
     n,1,Ring,Ring1,c,2,(N),x,N,3,C,4,(=0),x,c,4a,Ring,Ring2,n,5,c,6,c,7,n,8,c,8a,Rin
     q,Ring2,Ring,Ring1
     aminopterin root root
     0,10x,C(CCC(C(0)=0)NC(C3=CC=C(C=C3)NCC1=CN=C2C(C(N)=NC(N)=N2)=N1)=0)=0,x
     vitaminh root root O=C(N2)NC1C2CS[C@H]1CCCCC(O)=O,x
     brucine root root
     0=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCC5[C@]34[H])C1=C2C=C(OC)C
     (OC) = C1, x
     struchnine root root
     O=C(C5)N(C4[C@@]2(CC7)[C@](N7C6)([H])C[C@@]3([H])C6=CCC5[C@]34[H])C1=C2C=,x,C,1
     0, C, 11, = C1, x
     penicillan root root
     C,x,[C@@H],3,Ring,Ring2,N,4,Ring,Ring1,C,5,(,x,[C@H],6,([H]),x,[C@@],6a,Ring,Rin
     g1,([H]),x,S,1,C,2,Ring,Ring2,(C)C)=0,x
```

```
cephalosporan root root
C,x,C,4, Ring, Ring1,=,x,C,3, (COC(C)=0),x,C,2,S,1,[C@@],7a,(,x,[C@H],7,Ring,Ring2,
[H], x, y, x, ([H]), x, N, 5, Ring, Ring1, C, 6, Ring, Ring2, =0, x
vitaminb1|thiamine|thiamin|thiaminechloride|thiaminchlorid root root
O3.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[Cl-], x
vitaminb1nitrate | thiaminenitrate | thiaminnitrate root root
03.NC1=C(C[N+]2=CSC(CC3)=C2C)C=NC(C)=N1.[O-][N+]([O-])=O, \times C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=C2C(C3)=
thiaminedisulfide root root
 \texttt{CC} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC1} = \texttt{CN=C} \left( \texttt{N=C1N} \right) \texttt{C} \right) = \texttt{C} \left( \texttt{SSC} \left( \texttt{CCO} \right) = \texttt{C} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC2} = \texttt{C} \left( \texttt{N} \right) \texttt{N=C} \left( \texttt{C} \right) \texttt{N=C2} \right) \texttt{C} \right) \texttt{CCO}, \\ \texttt{x} = \texttt{CC} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC1} = \texttt{CN=C} \left( \texttt{N-C1N} \right) \texttt{C} \right) = \texttt{C} \left( \texttt{SSC} \left( \texttt{CCO} \right) = \texttt{C} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC2} = \texttt{C} \left( \texttt{N} \right) \texttt{N=C} \left( \texttt{C} \right) \texttt{N=C2} \right) \texttt{C} \right) \\ \texttt{CC} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC1} = \texttt{CN=C} \left( \texttt{N-C1N} \right) \texttt{C} \right) = \texttt{C} \left( \texttt{SSC} \left( \texttt{CCO} \right) = \texttt{C} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC2} = \texttt{C} \left( \texttt{N} \right) \texttt{N=C} \right) \texttt{C} \right) \\ \texttt{CC} \left( \texttt{N} \left( \texttt{C=0} \right) \texttt{CC1} = \texttt{CN=C} \right) + \texttt{C} \left( \texttt{N-C1N} \right) \texttt{CC2} + \texttt{C} \left( \texttt{N-C1N} \right) + \texttt{C} \left( \texttt{N-C1N}
vitaminb2 riboflavin root root
 \texttt{CC1=CC2=C} \ (\texttt{N=C} \ (\texttt{C} \ (\texttt{N3}) = \texttt{O}) \ (\texttt{N2C} \ [\texttt{C@eH}] \ (\texttt{O}) \ [\texttt{C@eH}] \ (\texttt{O}) \ (\texttt{C@eH}] \ (\texttt{O}) \ , \\ \texttt{x}, \texttt{C}, \texttt{5}', \texttt{O}) = \texttt{NC3} = \texttt{O}) \ \texttt{C=C1C}, \\ \texttt{x}, \texttt{y}, \texttt{y},
vitamine alphatocopherol atocopherol root root
CC1 = C2C(0[C@@](CCC[C@H](C)CCC[C@H](C)CCC[C@H](C)C)(C)CC2) = C(C)C(C) = C10, \times C100, \times C10, \times C10, \times C10
phenolsulfonphthalein phenolsulfonephthalein root root
C,1,Ring,Ring1,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2, Ring, Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,0,x,),x,c,5',c,6',Ri
ng,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,0,x,),x,c,5'',c,6'',Ring,Rin
q4
mcresolsulfonphthalein | mcresolsulfonephthalein root root
C,1,Ring,Ring1,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2, Ring, Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(0),x,c,3',c,4',(,x,C,x,),x,c,5',c
  ,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(0),x,c,3'',c,4'',(,x,C,x,),x,c,5'',c,
 6'', Ring, Ring4
ocresolsulfonphthalein ocresolsulfonephthalein root root
C,1,Ring,Ring1,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
Ring2, Ring1, ), x, (,x,c,1', Ring, Ring3,c,2',c,3',(0),x,c,4',(,x,C,x,),x,c,5',c
  ,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(0),x,c,4'',(,x,C,x,),x,c,5'',c,
 6'', Ring, Ring4
pyrocatecholsulfonphthalein|pyrocatecholsulfonephthalein root root
C,1,Ring,Ring1,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2, Ring, Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(,x,0,x,),x,c,5',c
  ,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(0),x,c,4'',(,x,0,x,),x,c,5'',c,
  6'', Ring, Ring4
pyrogallolsulfonphthalein|pyrogallolsulfonephthalein root root
C, 1, Ring, Ring1, (x, 0, 2, 5, 3, (=0), (=0), x, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring4, Ring5, Ring5, C, 1, Ring6, R
 Ring2, Ring, Ring1, ), x, (,x,c,1',Ring,Ring3,c,2',(,x,0,x,),x,c,3',(0),x,c,4',(,x,0,
x,),x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,0,x,),x,c,3'',(0),x,c,
 4'', (,x,0,x,),x,c,5'',c,6'',Ring,Ring4
  thymolsulfonphthalein|thymolsulfonephthalein root root
 C,1,Ring,Ring1,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,
 Ring2, Ring, Ring1, x, (x, c, 1', Ring, Ring3, c, 2', (x, C(C)C, x,), x, c, 3', c, 4', (x, 0, x, c, 2', c, 4', c, 2', c
  ),x,c,5',(C),x,c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,C(C)C,x,),x,c,3'',
  c,4'',(,x,0,x,),x,c,5'',(C),x,c,6'',Ring,Ring4
  phenolphthalein root root
  C,1,Ring,Ring1,(,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
  2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,0,x,),x,c,5',c,6',Ring,R
  ing3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,0,x,),x,c,5'',c,6'',Ring,Ring4
  mcresolphthalein root root
  C, 1, Ring, Ring1, (,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
  2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(0),x,c,3',c,4',(,x,C,x,),x,c,5',c,6',
  Ring, Ring3,),x,c,1'',Ring,Ring4,c,2'',(0),x,c,3'',c,4'',(,x,C,x,),x,c,5'',c,6'',
  Ring, Ring4
  ocresolphthalein root root
  2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(,x,C,x,),x,c,5',c,6',
  Ring, Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',(0),x,c,4'',(,x,C,x,),x,c,5'',c,6'',
  Ring, Ring4
```

```
pyrocatecholphthalein root root
c, 1, Ring, Ring1, (,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',(0),x,c,4',(,x,0,x,),x,c,5',c,6',
Ring, Ring3, ), x,c,1'', Ring, Ring4,c,2'',c,3'',(0),x,c,4'',(,x,0,x,),x,c,5'',c,6'',
Ring, Ring4
pyrogallolphthalein root root
C, 1, Ring, Ring1, (,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',(,x,0,x,),x,c,3',(0),x,c,4',(,x,0,x,),
x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,0,x,),x,c,3'',(0),x,c,4'',
(,x,0,x,),x,c,5'',c,6'',Ring,Ring4
thymolphthalein root root
C,1,Ring,Ring1,(,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
c,5',(C),x,c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',(,x,C(C)C,x,),x,c,3'',c,4'
 ',(,x,0,x,),x,c,5'',(C),x,c,6'',Ring,Ring4
tetraiodophthalein|iodophthalein|iodophene|iodotetragnost root root
C,1,Ring,Ring1,(,x,0,2,C,3,(=0),x,c,3a,Ring,Ring2,c,4,(I),x,c,5,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,(I),x,c,6,
c,7,(I),x,c,7a,Ring,Ring2,Ring,Ring1,),x,(,x,c,1',Ring,Ring3,c,2',c,3',c,4',(,x,
0,x,),x,c,5',c,6',Ring,Ring3,),x,c,1'',Ring,Ring4,c,2'',c,3'',c,4'',(,x,0,x,),x,
c,5'',c,6'',Ring,Ring4
fluorescein root root
a, Ring, Ring2, Ring1, ), x, c, 10a, Ring, Ring3, c, 1', c, 2', c, 3', (,x,0,x,), x, c, 4', c, 4
a',Ring,Ring3,0,x,c,5b',Ring,Ring4,c,5',c,6',(,x,0,x,),x,c,7',c,8',c,8a',Ring,Ri
ng5, Ring, Ring4
sulfonfluorescein root root
c,1,Ring,Ring1,Ring,Ring5,(,x,0,2,S,3,(=0)(=0),x,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7
,c,7a,Ring,Ring2,Ring,Ring1,),x,c,10a,Ring,Ring3,c,1',c,2',c,3',(,x,0,x,),x,c,4'
,c,4a',Ring,Ring3,0,x,c,5b',Ring,Ring4,c,5',c,6',(,x,0,x,),x,c,7',c,8',c,8a',Rin
g, Ring5, Ring, Ring4
fluoran fluorane root root
a, Ring, Ring2, Ring, Ring1,), x, c, 10a, Ring, Ring3, c, 1', c, 2', c, 3', c, 4', c, 4a', Ring, Ring
3,0,x,c,5b',Ring,Ring4,c,5',c,6',c,7',c,8',c,8a',Ring,Ring5,Ring,Ring4
uramil root root N,n,C1C(=0)NC(=0)NC(=0)1,x
isosorbide root root
O,x,[C@H],2,Ring,Ring1,C,1,O,x,[C@@],4,Ring,Ring2,(,x,[H],x,),x,[C@],3,Ring,Ring
1, (x, [H], x, x, x, 0, x, C, 6, [C@H], 5, Ring, Ring2, 0, x
isoproterenol|isoprenaline root root CC(NCC(C1=CC(0)=C(0)C=C1)0)C,x
shikonin root root CC(C) = CC[C@@H](O)C(C(c1c(O)ccc(O)c12)=0) = CC2=0, x
alkannin root root CC(C)=CC[C@H](O)C(C(c1c(O)ccc(O)c12)=O)=CC2=O, x
shikalkin root root CC(C)=CCC(0)C(C(c1c(0)ccc(0)c12)=0)=CC2=0,x
hyoscyamine root root CN1C2CCC1C[C@H](OC(C(CO)c3ccccc3)=O)C2,x
44'carbocyanine|cryptocyanine|kryptocyanine root root
 [n+],1,Ring,Ring1,c,2,c,3,c,4,(,x,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,c,8a,Ring,Ring
2,Ring,Ring1,),x,C=CC=,x,C,4',Ring,Ring3,C,3',=,x,C,2',N,1',c,8a',Ring,Ring4,c,8
 ',c,7',c,6',c,5',c,4a',Ring,Ring4,Ring,Ring3
22'carbocyanine|pinacyanol root root
 2,Ring,Ring1,),x,C=CC=,x,C,2',(,x,C,3',=,x,C,4',Ring,Ring3,),x,N,1',c,8a',Ring,R
 ing4,c,8',c,7',c,6',c,5',c,4a',Ring,Ring4,Ring,Ring3
oxacarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
 ',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
oxadicarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
```

```
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
oxatricarbocyanine root root
o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,0,1',Ring,Ring3
thiacyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c
,7a',Ring,Ring4,S,1',Ring,Ring3
thiacarbocyanine root root
s,1,Rinq,Rinq1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiadicarbocyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
ng,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
thiatricarbocyanine root root
s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
nq,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
selenacarbocyanine root root
[se],1,Ring,Ring1,cC,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
2,Ring,Ring1,),x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4'
,c,5',c,6',c,7',c,7a',Ring,Ring4,[Se],1',Ring,Ring3
hordenine root root CN(C)CCC1=CC=C(O)C=C1,x
maltol root root o1ccc(=0)c(0)c(C)1,x
coman root root Cc1=cc(=0)cco1,x
chrysoidine root root
c,4|p|para,(,x,c,3|m|meta,c,2|o|ortho,Ring,Ring1,),x,c,5,c,6,c,1,Ring,Ring1,N=Nc
2c(N)cc(N)cc2,x
alphafuril root root O=C(C1=CC=CO1)C(C2=CC=CO2)=O,x
anisil root root O=C(C1=CC=C(OC)C=C1)C(C2=CC=C(OC)C=C2)=O,x
alphaphellandrene root root CC1=CCC(C(C)C)C=C1,x
betaphellandrene root root CC(C(C=C1)CCC1=C)C, x
scopolamine scopolamin root root C[N+]1([0-
]) C2CCC1CC (OC (C (CO) C3 = CC = CC = C3) = O) C2, x
pilocarpine|pilocarpin root root CC[C@H]1[C@@H](CC2=CN=CN2C)COC1=0,x
quanethidine root root NC (NCCN1CCCCCCC1) = N, x
lobeline root root CN1C(CC(C3=CC=CC=C3)O)CCCC1CC(C2=CC=CC=C2)=O,x
mercaptur root root C[C@H](CS)NC(C)=O,x
phenylmercaptur root root C[C@H](CSc1ccccc1)NC(C)=0,x
alphalip alip root root CCCCCC1SSCC1,x
perill | perilla root root CC1=CCC(C(C)=C)CC1, x
biotin root root 0,1@x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
biotinyl root root C,40x,(CCCC[C0H]1[C0](NC2=O)([H])[C0](N2)([H])CS1)=O,x
biotinamide|biotinamid root root
N, x, C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O, x
bisphenola root root
01.0c,4,Ring,Ring2,c,5,c,6,c,1,(,x,c,2,c,3,Ring,Ring2,),x,C(C)(C),x,c,1',Ring,Ri
ng3,c,2',c,3',c,4',Ring,Ring1,c,5',c,6',Ring,Ring3
pantothen root root CCCNC(C(C(CO)(C)C)O)=O,x
alloxan root root
N, 1, Rinq, Ring1, C, 2, (=0), x, N, 3, C, 4, (=0), x, C, 5, (=0), x, C, 6, (=0), x, Ring, Ring1
croman root root Ccloccc(=0)cl,x
```

```
cinchon root root
C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
Ring4, n, 1' | a-1, c, 2' | a-b, c, 3' | a-
t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,=,x,C,11,)C3C1,x
1011dihydrocinchon root root
C,9,(,x,c,4',Ring,Ring2,c,4a',(,x,c,5',c,6',c,7',c,8',Ring,Ring4,),x,c,8a',Ring,
Ring4, n, 1' | a-1, c, 2' | a-b, c, 3' | a-
t,Ring,Ring2,),x,C,8,Ring,Ring1,N(CC3)CC(,x,C,10,C,11,)C3C1,x
cinchonine | cinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1, x
1011dihydrocinchonine | 1011dihydrocinchonin root root
O[C@@H]([C@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1, x
quinidine root root
O[C@@H]([C@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroguinidine root root
O[C@H]([C@H]2N(CC4)C[C@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1, \times O[C@H]([C@H]2N(CC4)C[C@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1, \times O[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[C@H](CC4)C[CG4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CG4](CC4)C[CC4](CC4)C[CG4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC4](CC4)C[CC
cinchonidine cinchonidin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=CC=C3)C3=NC=C1, x
1011dihydrocinchonidine | 1011dihydrocinchonidin root root
quinine quinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](C=C)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1,x
1011dihydroquinine | 1011dihydroquinin | dihydroquinine | dihydroquinin | hydroquinine | h
vdroquinin root root
O[C@H]([C@@H]2N(CC4)C[C@@H](CC)[C@]([H])4C2)C1=C(C=C(OC)C=C3)C3=NC=C1, x
hepes root root S, x, (=, x, 0, x,) (, x, =0, x,) (, x, 0, 1@0,), x, CCN(CC1)CCN1CCO, x
pipes root root O=S(CCN1CCN(CCS(=0)(0)=0)CC1)(0)=0, x
popop root root C1(C2=CC=C(C4=NC=C(C5=CC=CC=C5)O4)C=C2)=NC=C(C3=CC=CC=C3)O1,x
dibenzosuber root root
c,1,Ring,Ring1,c,2,c,3,c,4,c,4a,Ring,Ring2,C,5,c,5a,Ring,Ring3,c,6,c,7,c,8,c,9,c
,9a,Ring,Ring3,C,10,C,11,c,11a,Ring,Ring2,Ring,Ring1
benzosuber root root
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,c,5a,Ring,Ring2,c,6,c,7,c,8,c,9,c,9a,Ring,Ring2,R
ing, Ring1
orthosilicate root root
[Si], x, (,x,0,1@o''',), x, (,x,0,1@o'',), x, (,x,0,1@o',), x,0,1@o'
orthotitanate root root
[Ti], x, (,x,0,1@o''',), x, (,x,0,1@o'',), x, (,x,0,1@o',), x,0,1@o')
gona gon root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,C,17,C,13,Ring,Ring4,C,12,C,11,C,9,Ring,Ring3,C,10,Ring,Ring1
,Ring,Ring2
estra|oestra|estr|oestr root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3
,C,10,Ring,Ring1,Ring,Ring2
equilen root steroid
c,3,(0)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
 Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring_{x}Ring
Ring, Ring3, c, 10, Ring, Ring1, Ring, Ring2
dihydroequilen root steroid
c,3,(0)(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,c,6,c,7,c,8,Ring,Ring3,C,14
 Ring, Ring4, C, 15, C, 16, C, 17, (0), x, [C@@], 13, Ring, Ring4, (,x,C,x,), x,C,12,C,11,c,9,R
ing, Ring3, c, 10, Ring, Ring1, Ring, Ring2
androsta|androst|etiochola|etiochol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
```

```
ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring
3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
etioallochola etioallochol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etien root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
etian root steroid
c,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,
Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
androstenediol root steroid
[C@H], 3, (0), x, (,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@H],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x
,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
androstenedione root steroid
(x, 0), (x, 
ng3,C,14,Ring,Ring4,C,15,C,16,C,17,(=0),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,
C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
pregna pregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,
12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
allopregna allopregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,),x,[C@@],13,Ring,Ring4,(,x
,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
chola chol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[C@@],1
3,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring
2,C,19
cholesta cholest coprost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,2
7,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],1
0, Ring, Ring1, Ring, Ring2, C, 19
lanosta lanost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,[C@],4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@],2
0,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x
,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dammara dammar root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,[C@],4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@],
20, (x, C, 22, C, 23, C, 24, C, 25, (x, C, 26,), x, C, 27,), x, C, 21,), x, [C@@], 13, Ring, Ring4, C,
12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
urs root steroid
C, 3, (x, C, 2, C, 1, Ring, Ring1,), x, C, 4, (x, C, x,) (x, C, x,), x, C, 5, Ring, Ring2, C, 6, C, 7, [
C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C),
28,C,22,C,21,[C@@H],20,(,x,C,30,),x,[C@H],19,(,x,C,29,),x,[C@@],18,([H]),x,Ring,
Ring5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1,Ring,Ring2,C,x
```





lup root steroid C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C), 28,C,22,C,21,[C@@H],19,(,x,C,20,(,x,C,29,),x,C,30,),x,[C@@],18,([H]),x,Ring,Ring 5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1 ,Ring,Ring2,C,x taraxaster root steroid C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,x,)(,x,C,x,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,x,C,x,[C@@],x,Ring,Ring5 (C), 28, C, 22, C, 21, C, 20, (=,x,C,30,), x, (x,C,19,(,x,C,29,)), x, (C@], 18, ([H]), x, Ring, Ring 5, [C@@], 13, Ring, Ring4, (,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1 ,Ring,Ring2,C,x oleane olean root steroid C,3,(x,C,2,C,1,Ring,Ring1,),x,C,4,(x,C,23,)(x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,15,C,16,[C@@],x,Ring,R ing5, (C), 28, C, 22, C, 21, C, 20, (,x,C,30,) (,x,C,29,),x,C,x, [C@@], 18, ([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,(,x,[H],x,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1 ,Ring,Ring2,C,19 olean loveracid steroid C,x,Ring,Ring6,.,x,C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,23,)(,x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,),x,C,15, C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,C,x,(,x,C,x,)(,x,C,29,),x,C,x,[C@],x, ([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,=,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Rin g, Ring1, Ring, Ring2, C, 19 olean oleanol loveracid steroid C,x,Ring,Ring6,.,x,[C@H],3,(0)(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,23,)(,x,C,24,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,), x,C,15,C,16,[C@@],x,Ring,Ring5,Ring,Ring6,C,x,C,x,(,x,C,x,)(,x,C,29,),x,C,x, [C@],x,([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4, =,x,C,12,C,11,C,9,Ring,Ring3,[C@@] ,10,Ring,Ring1,Ring,Ring2,C,19 glycyrrhetin root steroid C, 29, Ring, Ring6, ..., x, [C@], 3, (0), x, (,x,C,2,C,1,Ring,Ring1,),x,C,4, (,x,C,x,) (,x,C,x,0),),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,) ,x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(,x,C,30,),x,Ring,Ring6,C x, [C@@], 18, ([H]), x, Ring, Ring5, C, 13, Ring, Ring4, =, x, C, 12, C, 11, (=0), x, C, 9, Ring, Rin q3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19 glycyrrhet root steroid ,),x,C,5,Ring,Ring2,C,6,C,7,[C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,x,) ,x,C,x,C,x,[C@@],x,Ring,Ring5,(C),28,C,22,C,21,[C@],20,(,x,C,30,),x,Ring,Ring6,C x, [C@@], 18, ([H]), x, Ring, Ring5, C, 13, Ring, Ring4, =, x, C, 12, C, 11, (=0), x, C, 9, Ring, Ring5, C, 13, Ring4, =, x, C, 12, C, 11, (=0), x, C, 9, Ring5, g3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19 solanid root steroid C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,[C@],8,([H]),x,Ring,Ri ng3,[C@@],14,([H]),x,Ring,Ring4,C,15,[C@@],16,([H]),x,Ring,Ring5,N,28,Ring,Ring6 ,C,x,[C@@],25,(C),x,C,24,C,23,[C@@],22,([H]),x,Ring,Ring6,[C@@],x,(C),x,[C@@],x, ([H]),x,Ring,Ring5,[C@@],13,Ring,Ring4,(C),18,C,12,C,11,C,9,Ring,Ring3,[C@@],10, Ring, Ring1, Ring, Ring2, C, x cholester root steroid

C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19

lanoster root steroid

C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,(,x,C,28,)(,x,C,29,),x,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,30,),x,C,15,C,16,[C@],17,(,x,[C@@H]

```
,20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(
,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
ergosta ergost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C),x,C,25,(,x,C,
26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin
g3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
campesta campest root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@@H],24,(C),x,C,25,(,x,C
,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri
ng3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
poriferasta poriferast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(CC),x,C,25,(,x,C
,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ri
ng3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
stigmasta|stigmast root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@@H],24,(,x,C,28,C,29,),
x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11
,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
pregnenolone root steroid
C,1,Ring,Ring1,C,2,C,3,(0),x,C,4,c,5,Ring,Ring2,c,6,C,7,C,8,Ring,Ring3,C,14,Ring
Ring4,C,15,C,16,[C@],17,(,x,C,20,(=0),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,)
,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
prednisolone prednisolon root steroid
C,1,Ring,Ring1,=,x,C,2,C,3,(=0),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,
C, 14, Ring, Ring 4, C, 15, C, 16, [C@@], 17, (,x,C,20, (=0), x,C,21,0,x,),x, (,x,0,x,),x, [C@@]
],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,(,x,0,x,),x,C,9,Ring,Ring3,[C@@],10,Ring,
Ring1, Ring, Ring2, C, 19
progesterone progesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(=0),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin
q, Rinq4, C, 15, C, 16, [C@], 17, (,x,C,20, (=0),x,C,21,),x, [C@@], 13, Ring, Ring4, (,x,C,18,
),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
tetrahydroprogesterone tetrahydroprogesteron root steroid
C,1,Ring,Ring1,C,2,C,3,(0),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ring
Ring4,C,15,C,16,[C@],17,(,x,C,20,(0),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),
x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
hydrocortisone hydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=0),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
Ring, Ring, C, 15, C, 16, [C@@], 17, (,x,C,20, (=0),x,C,21,0,x,),x, (,x,0,x,),x, [C@@], 13
Ring, Ring4, (,x,C,18,),x,C,12, [C@@H],11,(0),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
dihydrocortisone dihydrocortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=0),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Rin
g,Ring4,C,15,C,16,[C@@],17,(,x,C,20,(=0),x,C,21,0,x,),x,(,x,0,x,),x,[C@@],13,Rin
g,Ring4,(,x,C,18,),x,C,12,[C@@H],11,(=0),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ri
ng, Ring2, C, 19
tetrahydrocortisone tetrahydrocortison root steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
, Ring, Ring4, C, 15, C, 16, [C@@], 17, (,x,C,20, (=0),x,C,21,0,x,),x, (,x,0,x,),x, [C@@], 13
Ring, Ring4, (,x,C,18,),x,C,12, [C@@H],11,(0),x,C,9,Ring,Ring3, [C@@],10,Ring,Ring1
,Ring,Ring2,C,19
cortisone cortison root steroid
C,1,Ring,Ring1,C,2,C,3,(=0),x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
, Ring, Ring4, C, 15, C, 16, [C@@], 17, (,x,C,20, (=0),x,C,21,0,x,),x, (,x,0,x,),x, [C@@], 13
```

```
Ring, Ring4, (,x,C,18,),x,C,12, [C@@H],11, (=0),x,C,9,Ring,Ring3, [C@@],10,Ring,Ring,
1, Ring, Ring2, C, 19
androsterone root steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
Ring, Ring4, C, 15, C, 16, C, 17, (=0), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9
,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
isoandrosterone root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,
Ring, Ring4, C, 15, C, 16, C, 17, (=0), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, C,12,C,11,C,9, C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,11,C,12,C,12,C,11,C,12,C,12,C,11,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,12,C,1
Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
aldosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=0),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,0,x,),x,[C@@],13,Ring,Ring4,(,x,C,1
8,=0,x,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,1
pregnanolone root steroid
C,3,(0)(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
 , Ring, Ring4, C, 15, C, 16, [C@], 17, (,x,C,20, (=0),x,C,21,),x, [C@@], 13, Ring, Ring4, (,x,C,21,),x, [C@@], (,x,C,21,),x, [C@], (,x,C,21,),x, [C@], (,x,C,21,),x, [C@], (,x,C,21,),x, [C@], (,x,C,21,),x, (,x,C,21,),x, (,x,C,21,),x, (,x
,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
testosteron testosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=0),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
dihydrotestosteron dihydrotestosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=0),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
oestradiol estradiol betaestradiol petaestradiol root steroid
c,3,(0),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11
 ,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestriol estriol root steroid
c,3,(0),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,[C@@],16,(O),x,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x
 ,C,12,C,11,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestrone estrone root steroid
c,3,(0),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
 ,14,Ring,Ring4,C,15,C,16,C,17,(=0),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C
,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
brassinolid brassinolide root steroid
 [C@@H],3,(0),x,(,x,[C@H],2,(0),x,C,1,Ring,Ring1,),x,C,4,[C@],5,Ring,Ring2,([H]),
x,C,6,(=0)0,x,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,
 (x, [C@H], 22, (0), x, [C@H], 23, (0), x, [C@@H], 24, (0), x, C, 25, (x, C, 26,), x, C, 27,), x, C, 2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
calcidiol root root
 [C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (,x, [C@@], 20, (,x,C, 22, C, 23, C, 24, C, 2
5, (,x,C,26,)(0),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
 ,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
calciol|cholecalciferol|vitamind3 root root
 [C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8
r,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C
 ,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11|a-
 t,C,9|a-b,Ring,Ring3,...,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
```

,10,Ring,Ring1,Ring,Ring2,C,19

```
calcitriol root root
[C@H], 3, (0), x, (,x,C,2,[C@H],1,(0),x,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,
7,=,x,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,2
3,C,24,C,25,(,x,C,26,)(0),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C
,12,C,11,C,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
corticosterone root steroid
C,3,(=0)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=0),x,C,21,0,x,),x,[C@@],13,Ring,Ring4,
(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C
cortisol root steroid
C,3,(=0)(,x,C,2,C,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4, Ring, Ring4, C, 15, C, 16, [C@], 17, (,x,C,20, (=0),x,C,21,0,x,)(0),x,[C@@], 13, Ring, Rin
q4,(,x,C,18,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring
2,C,19
ecdysone root steroid
[C@H],3,(O),x,(,x,[C@@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H])
x,C,6,(=0),x,C,7,=,x,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(0),x,C,15,C,16,[C@],17,
(x, \{C@@\}, 20, (x, C, 22, (0), x, C, 23, C, 24, C, 25, (0), x, C, 26, ), x, C, 27, ), x, C, 21, ), x, [C@]
@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,
Ring2,C,19
ercalciol|ergocalciferol root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,=,x,C,23,[C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C,12,C,11,C,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
ergosterol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (,x, [C@@], 20, (,x,C, 22, =,x,C, 23, [C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
lumisterol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (,x, [C@@], 20, (,x,C, 22, =,x,C, 23, [C@H
],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,
C,12,C,11,[C@],9,([H]),x,Ring,Ring3,[C@],10,Ring,Ring1,Ring,Ring2,C,19
cardanolide root steroid
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,23,(=0),x,C,22,Rin
g,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,R
ing, Ring1, Ring, Ring2, C, 19
card2022enolide 2022cardenolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,C,20,Ring,Ring5,C,21,0,x,C,23,(=0),x,C,22,=,x,Rin
g,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,R
ing, Ring1, Ring, Ring2, C, 19
digitoxigenin root steroid
0,x,[C@@],3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@],5,Ring,Ring2,([H]),x,C,6,C,7,C,
8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (,x,C,20, Ring, Ring5, C, 21, 0, x, C, 23
,(=0),x,C,22,=,x,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,R
ing, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
bufanolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,C,21,O,x,C,24,(=0),x,C,23,C,2
2,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@]
```

ing2,C,19

```
bufadienolide root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,Ring,Ring5,=,x,C,21,0,x,C,24,(=0),x,C,23
,=,x,C,22,Ring,Ring5,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Rin
g3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
cev root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,[C@@],1
4,([H]),x,Ring,Ring4,C,15,C,16,[C@@],17,([H]),x,Ring,Ring5,[C@@H],20,(C),x,[C@@]
x,([H]),x,Ring,Ring6,C,x,C,x,[C@H],x,(C),x,C,x,N,x,Ring,Ring6,C,x,[C@],x,([H]),
x,Ring,Ring5,[C@@],12,([H]),x,Ring,Ring4,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
solidan root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,Ring,Ring5,[C@],17,([H])(,x,[C@],20,(,x,C,21,),x,[C@],22,([H]
),x,Ring,Ring6,C,23,C,24,[C@H],25,(,x,C,27,),x,C,26,N,28,Ring,Ring6,Ring,Ring5,)
x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1
,Ring,Ring2,C,19
spirost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@@],20,(,x,
[C@@],22,Ring,Ring5,(,x,0,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),
x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C
@@],10,Ring,Ring1,Ring,Ring2,C,19
spirosol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
mg,Ring4,C,15,[C@],16,([H])(,x,0,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@],20,(,x,C)
,22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,C,25,(,x,C,26,Ring,Ring6,),x,C,2
7,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],1
0, Ring, Ring1, Ring, Ring2, C, 19
tomatid root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,
[C@],20,(,x,[C@],22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,[C@@H],25,(,x,C,
26,Ring,Ring6,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
solasod root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,[C@@H],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,
[C@],20,(,x,[C@@],22,Ring,Ring5,(,x,N,x,Ring,Ring6,),x,C,23,C,24,[C@H],25,(,x,C,
26, Ring, Ring6, ), x, C, 27, ), x, C, 21, ), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x, C, 12, C, 11, C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
furost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,[C@],16,([H])(,x,O,x,Ring,Ring5,),x,[C@],17,([H])(,x,[C@@],20,(,x,
[C@],22,Ring,Ring5,C,23,C,24,C,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,R
ing4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
chol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@]
,10,Ring,Ring1,Ring,Ring2,C,19
lithochol loveracid steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[C@@
],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,R
```

```
dehydrochol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,(=0),x,C,4,C,5,Ring,Ring2,C,6,C,7,(=0),x,C,8,Ring,Ring3,C
14,Ring,Ring4,C,15,C,16,[Ce],17,(,x,[CeeH],20,(,x,C,22,C,23,C,24,),x,C,21,),x,[
C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,(=0),x,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
hyodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,[C@@H],3,(O),x,C,4,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1, Ring, Ring2, C, 19
chenodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,[C@@H],4,(O),x,C,5,Ring,Ring2,C,6,[C@@H],7,(O),x,C,8,Ring
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,
21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1, Ring, Ring2, C, 19
ursodeoxychol loveracid steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,),x,C,21
,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Rin
g1, Ring, Ring2, C, 19
tauroursodeoxychol loveracid steroid
S, x, (=0), x, (=0), x, (x,0,10x,), x, C, x, C, x, N, x, Ring, Ring5, ..., x, C, 1, Ring, Ring1, C, 2, [C]
@@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,[C@H],7,(O),x,C,8,Ring,Ring3,C,14,Ring,Ring4
,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=0),x,Ring,Ring5,),x,C,21,)
x, [C@@], 13, Ring, Ring4, (,x,C,x,),x,C,12,C,11,C,9,Ring,Ring3, [C@@],10,Ring,Ring1,
Ring, Ring2, C, 19
taurochol loveracid steroid
S,x,(=0),x,(=0),x,(,x,0,10x,),x,C,x,C,x,N,x,Ring,Ring5,.,x,C,1,Ring,Ring1,C,2,C,
3, [C@H], 4, (O), x, C, 5, Ring, Ring2, C, 6, [C@@H], 7, (O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4
,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=0),x,Ring,Ring5,),x,C,21,)
x,[C@@],13,Ring,Ring4,(,x,C,x,),x,[C@@H],12,(O),x,C,11,C,9,Ring,Ring3,[C@@],10,
Ring, Ring1, Ring, Ring2, C, 19
glycochol loveracid steroid
C,1,Ring,Ring1,C,2,C,3,[C@H],4,(O),x,C,5,Ring,Ring2,[C@@H],6,(O),x,C,7,C,8,Ring,
Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,(=0)NCC
x,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,[C@@H],12,(O),x,C,11,C,9,Ring,R
ing3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19
oxymetholone root steroid
(x, 0), (x, 0, 2), (x, 0,
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(O)(C),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,
C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
homo natderiver nathomo x,x
nor natderiver natnor x,x
seco natderiver natseco x,x
abeo natderiver natabeo x,x
cyclo natderiver cyclo x,x
rightarrow|arrow|fwdarrow|fwdarw unknown natarrow x,x
flophemesyl root root [Si], 40x, (C)(C)c1c(F)c(F)c(F)c(F)c(F)1, x
diethylenetriamine root root N, n \mid 1, C, 2, C, 3, N, n' \mid 4, C, 5, C, 6, N, n' \mid 7
triethylenetetramine root root N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'
tetraethylenepentamine root root
N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n'
pentaethylenehexamine root root
N,n,CC,x,N,n'',CC,x,N,n''',CC,x,N,n'''',CC,x,N,n'''',CC,x,N,n'
cupferron root root O=NN([O-])c1ccccc1.[NH4+],x
camphene root root C=C(CC(CC2)C1(C)C)C12C,x
```

```
isopinocamphe root root
C,3,Ring,Ring1,C,4,C,5,(,x,C,6,Ring,Ring2,),x,C,7,(C)(C),x,C,1,Ring,Ring2,C,2,(C)
),x,Ring,Ring1
choline root root 0,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
phosphocholine root root 0,1@x,P,x,(=0),x,([0-
]),x,0,x,C,b| beta,C,a|alpha,[N+](C)(C)C,x
diphosphocholine root 0,10x,P,x,(=0),x,(,x,0,10x,),x,0,x,P,x,(=0),x,([0+x,0],x,0,x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,([0+x,0],x,0,x,P,x,(=0),x,([0+x,0],x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,([0+x,0],x,0,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x,x,P,x
]),x,0,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
phosphoethanolamine root root 0,10x,P,x,(=0),x,(0),x,0,x,C,b|beta,C,a|alpha,N,x
fluorocholine root root F,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
chlorocholine root root Cl,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
bromocholine root root Br,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
iodocholine root root I,x,C,b|beta,C,a|alpha,[N+](C)(C)C,x
betaine | betain root root [O-], x, C, x, (=0), x, C, a | alpha, [N+] (C) (C) C, x
betainealdehyde | betainaldehyd root root [H], x, C, x, (=0), x, C, a | alpha, [N+](C)(C)C, x | alph
carnitine carnitin root root 0,100,Ring,Ring1,.,x,[0-
], x, C, x, (=0), x, C, a alpha, C, b beta, Ring, Ring1, C, g gamma, [N+] (C) (C) C, x
carnitinamide root root
N, x, C, x, (=0), x, C, a | alpha, C, b | beta, (0), 1@o, C, g | gamma, [N+] (C) (C) C, x
aminocarnitine aminocarnitin root root [0-
 ], x, C, x, (=0), x, C, a alpha, C, b beta, (N), x, C, g gamma, [N+] (C) (C) C, x
exact-azine root root n1ccccc1,x
exact-ether root root CCOCC, x
exact-alcohol root root OCC, x
exact-salt root root [Na+].[Cl-],x
exact-sulfur root root S1SSSSSSS1,x
exact-phenazo root root OC(C=C4)=CC=C4N=NC(C([N+]([O-
 ]) = 0) = C2) = CC = C2C1 = CC([N+]([O-]) = 0) = C(N=NC3 = CC = C(0)C = C3)C = C1, x
\texttt{exact-nitron root } \texttt{C2}([\texttt{N-}]\texttt{N}(\texttt{C4=CC=CC=C4})\texttt{C=}[\texttt{N+}]\texttt{2C3=CC=CC=C3}) = \texttt{NC1=CC=CC=C1}, \texttt{X}(\texttt{N-})\texttt{NC1=CC=CC=C1}, \texttt{X}(\texttt{N-})\texttt{NC1=CC=CC=C1}) = \texttt{NC1=CC=CC=C1}, \texttt{NC1=CC=C1}, \texttt{NC1=CC=C1}, \texttt{NC1=CC=C1}, \texttt{NC1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1=C1}, \texttt{NC1=C1=C1}, \texttt{NC1=C1=C1
exact-anthranil root root clonc2cccc12,x
exact-acetal root root CC(OCC)OCC,x
 exact-sugar root root
OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO
)02,x
 exact-bisacrylamide root root O=C(C=C)NCNC(C=C)=O, x
 exact-dopa root root
 C,1,Ring,Ring1,.,x,N,n|nalpha|n2,C,a|alpha,Ring,Ring1,C,b|beta,c,x,Ring,Ring2,c,
 2|o|ortho,c,3|m|meta,(0),x,c,4|p|para,(0),x,c,5,c,6,Ring,Ring2
 exact-hydrogen root root [H][H],x
 exact-deuterium root root [2H][2H], x
 zincon root root
 O[S] (=0) (C1=CC(N=NC(C3=CC=CC=C3)=NNC2=CC=C2C(0)=0)=C(0)C=C1)=0,×
 chloroform root chloroform C([H])(Cl)(Cl)Cl,x
 fluoroform root chloroform C([H])(F)(F)F,X
 bromoform root chloroform C([H])(Br)(Br)Br,x
 iodoform root chloroform C([H])(I)(I)I,x
  ferricyanide root root [Fe-3](C#N)(C#N)(C#N)(C#N)(C#N)(C#N), x
  ferrocvanide root root [Fe-4](C#N)(C#N)(C#N)(C#N)(C#N)(C#N), x
 dibromochloride root root [Cl-](Br)Br,x
 dibromoiodide root root [I-](Br)Br,x
 dichloroiodate dichloroiodide root root [I-](Cl)Cl,x
 diiodoaurate root root [Au-](I)I,x
 dichloroaurate root root [Au-](Cl)Cl,x
  dibromoaurate root root [Au-](Br)Br,x
  bromodiiodide root root [Br-](I)I,x
  dichlorobromide root root [Br-](Cl)Cl,x
```

ű

:: :**:}**u

2

1

"Li

. Ž

L

```
tetrachloroiodate|iodotetrachloride root root [I-](Cl)(Cl)(Cl)Cl,x
chlorochromate root root [0-][Cr](=0)(=0)Cl,x
fluorochromate root root [O-][Cr](=O)(=O)F,x
fluoroborate|fluoroborat|tetrafluoroborate|tetrafluoroborate1|tetrafluoroborat|b
f4|borofluoride|borofluorid|fluoborate|fluoborat root root [B-](F)(F)(F)F,x
fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat root root [Si-
- ] (F) (F) (F) (F) (F) F, x
borohydride|borohydrid root root [B-],x
borodeuteride | borodeuterid root root [B-]([2H])([2H])([2H])[2H],x
cyanoborodeuteride | cyanoborodeuterid root root [B-]([2H])([2H])([2H])C#N,x
aluminohydride aluminohydrid root root [Al-], x
persulfate|persulfat|peroxodisulfate|peroxodisulfat root root
0,10x,S(=0)(=0)00S(=0)(=0),x,0,10x
bifluoride|bifluorid root root [F-],x,.[H]F,x
water root root [H]O[H],x
hydrofluoride root hydrochloride [H]F,x
hydrochloride | hcl root hydrochloride [H]Cl,x
2hcl root hydrochloride [H]Cl.[H]Cl,x
3hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl,x
4hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl,x
5hcl root hydrochloride [H]Cl.[H]Cl.[H]Cl.[H]Cl.[H]Cl,x
methochloride chlormethylate root hydrochloride CCl,x
methobromide brommethylate root hydrochloride CBr, x
hydrobromide | hbr root hydrochloride [H]Br, x
2hbr root hydrochloride [H]Br.[H]Br,x
3hbr root hydrochloride [H]Br.[H]Br.[H]Br,x
4hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br,x
5hbr root hydrochloride [H]Br.[H]Br.[H]Br.[H]Br.[H]Br,x
hydrotribromide|hbr root hydrochloride [H]Br(Br)Br,x
hydroiodide|hydriodide root hydrochloride [H]I,x
methoiodide methiodide root hydrochloride CI, x
ethoiodide ethiodide root hydrochloride CCI,x
hydrate|h2o root hydrochloride [H]O[H],x
deuterate d2o root hydrochloride [2H]O[2H], x
etherate root hydrochloride
O(C([H])([H])C([H])([H])[H])C([H])([H])([H])([H])([H])[H], \times
bitartarate|bitartrate|hydrogentartrate root hydrochloride
0,10x,C,1,(=,x,0,x,),x,C,2,(,x,0,x,),x,C,3,(,x,0,x,),x,C,4,(=,x,0),x,0,x,[H],x
dbitartrate hydrogendtartrate root hydrochloride
lbitartrate|hydrogenltartrate root hydrochloride
0.10x, C.1, (=,x,0,x,), x, [C0H], 2, (,x,0,x,), x, [C00H], 3, (,x,0,x,), x, C.4, (=,x,0), x,0,
x, [H], x
bimaleate hydrogenmaleate root hydrochloride
0,1@x,C,1,(=,x,0,x,),x,/,x,C,2,=,x,C,3,\,x,C,4,(=,x,0),x,0,x,[H],x
bisuccinate hydrogensuccinate root hydrochloride
0.10x, C.1, (=, x, 0, x,), x, C.2, C.3, C.4, (=0)0[H], x
biphthalate root hydrochloride
0,10x,C(=0),x,c,1,Ring,Ring1,c,2,(C(=0)O[H]),x,c,3,c,4,c,5,c,6,Ring,Ring1
hydrogenoxalate root hydrochloride
0,10x,C,1,(=,x,0,x,),x,C,2,(=,x,0),x,0,x,[H],x
bisulfate|bisulfat|hydrogensulfate root root 0,1@x,S(=0)(=0)0[H],x
bisulfite|bisulfit|hydrogensulfite root root 0,1@x,S(=0)O[H],x
bisulfide|bisulfid|hydrogensulfide root root S,1@x,[H],x
glycol|cellosolve|cellosolv root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,O,1@x,.,x,O,1@x,Ring,Ring1
```

```
thioglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,.,x,O,1@x,Ring,Ring1
dithioglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,.,x,S,1@x,Ring,Ring1
selenoglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,.,x,0,1@x,Ring,Ring1
diselenoglycol root glycol
C, 1 | a | alpha, Ring, Ring1, C, 2 | b | beta, [Se], 1@x, .,x, [Se], 1@x, Ring, Ring1
telluroglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],10x,.,x,0,10x,Ring,Ring1
ditelluroglycol root glycol
C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,.,x,[Te],1@x,Ring,Ring1
tempo root root
C, 4, Ring, Ring1, C, 5, C, 6, (C)(C), x, N, 1, (, x, 0, 160x,), x, C, 2, (C)(C), x, C, 3, Ring, Ring1
proxyl root root
C, 3, Ring, Ring1, C, 2, (C) (C), x, N, 1, (,x,0,16ex,), x, C, 5, (C) (C), x, C, 4, Ring, Ring1
nitroxide nitroxyl root root N,n,O,160x
nitramine root root N,n,[N+](=0)[0-],x
nitramino root root N, 4@n, [N+] (=0) [O-], x
special-oxine root root
n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(0),x,c,8a,Ring
g, Ring1, Ring, Ring2
special-azine ketazine root azine N,80x,N,80x
oxime oxim antioxime root oxime N,8@x,0,0
hydrazone hydrazon root oxime N,8@x,N,n
semicarbazone|semicarbazon root oxime N,8@1,N,2,C,3,(=,x,0,x,),x,N,4
azino root bridge N,8@x,N,8@x
azimino root bridge N,4@x,N,x,=,x,N,4@x
biimino|biimin root bridge N,4@x,N,4@x
epidioxy root bridge 0,40x,0,40x
epidithio epidithi root bridge S,40x,S,40x
epimino root bridge N,5@x
epithio root bridge S,5@x
episeleno root bridge [Se],50x
epitelluro root bridge [Te],5@x
epithioximino|epithioximin root bridge S,40x,0,x,N,40x
epoxy root bridge 0,50x
epoxyimino epoxyimin root bridge 0,40x,N,40x
epoxynitrilo root bridge 0,40x,N,80x
epoxythio epoxythi root bridge 0,40x,S,40x
epoxythioxy root bridge 0,40x,S,x,0,40x
epitrithio|epitrithi root bridge S,40x,S,x,S,40x
cyanohydrin root oxime 0,40x,.,x,C,40x,#N,x
fluorohydrin root oxime 0,40x,.,x,F,40x
chlorohydrin root oxime 0,4@x,.,x,Cl,4@x
bromohydrin root oxime 0,4@x,.,x,Br,4@x
iodohydrin root oxime 0,40x,.,x,I,40x
acetal|ketal|semiacetal|demiacetal|hemiacetal|semiketal|demiketal|hemiketal|glyc
olacetal glycolketal root oxime 0,40x,.,x,0,40x
mercaptal mercaptole root oxime S,40x,.,x,S,40x
ketone keton root ketone C, x, =, x, 0, x
ketoxime root ketone C, x, =, x, N, x, 0, x
ketoximino root ketone C, x, =, x, N, x, O, 40x
ketyl root ketone C,40x,[0-],x
sulfoxide sulfoxid root ketone S, x, =, x, 0, x
sulfone sulfon root ketone S, x, (=,x,0,x,), x,=,x,0,x
sulfimide|sulfimid|sulfilimine|sulfilimin root ketone S,x,=,x,N,x
```

```
sulfoximide|sulfoximid|sulfoximine|sulfoximin root ketone
S, x, (=, x, 0, x,), x, =, x, N, x
selenoxide|selenoxid root ketone [Se],x,=,x,0,x
selenone selenon root ketone [Se], x, (=, x, 0, x,), x, =, x, 0, x
selenimide selenimid root ketone [Se], x, =, x, N, x
selenoximide selenoximid root ketone [Se], x, (=, x, 0, x, ), x, =, x, N, x
telluroxide telluroxid root ketone [Te],x,=,x,0,x
tellurone telluron root ketone [Te], x, (=, x, 0, x, ), x, =, x, 0, x
tellurimide tellurimid root ketone [Te],x,=,x,N,x
telluroximide|telluroximid root ketone [Te],x,(=,x,0,x,),x,=,x,N,x
peroxide peroxid root ketone 0,x,0,x
persulfide persulfid root ketone S,x,S,x
formal root ketone O,x,Ring,Ring1,.,x,O,x,C,x,Ring,Ring1
ether root ether 0,x
etherof root ofether O,x
thioether root ether S,x
selenoether root ether [Se],x
telluroether root ether [Te],x
oin oin unknown C,1@b|beta,(0),x,C,1@a|alpha,=0,x
ano methanomaker unknown x,x
quinone quinon suffix quinone 0,80x
quinodimethane | quinodimethan suffix quinone C, 10@x
radical radical unknown x,x
yl suffix yl 1,yl
ylidene|yliden|ilidene|iliden| suffix yl 2,yl
ylidyne|ylidyn|ilidyne|ilidyn suffix yl 3,yl
ane an suffix ignore x,x
ine in suffix ignore x,x
ene en suffix bondchange 2, bond
yne yn suffix bondchange 3,bond
thiol|ylthiol suffix suffix S,4@s
ol suffix olsuffix 0,40x
olate suffix suffix [0-],40x
anethiolate thiolato suffix suffix [S-],40x
one on suffix requarbon 0,80x
thione suffix regcarbon S,8@x
selenone | selone suffix requarbon [Se], 80x
tellurone suffix regcarbon [Te],80x
imine root oxime N,8@n
imine imine suffix N,8@n
iminium root oxime [N+],8@x
iminium imine suffix [N+],80x
glycol glycol unknown 0,400,..,x,0,400'
thioglycol glycol unknown S,4@s,.,x,0,4@o
dithioglycol glycol unknown S,4@s,.,x,S,4@s'
selenoglycol glycol unknown [Se], 40x,.,x,0,40x
diselenoglycol glycol unknown [Se], 40x,.,x,[Se], 40x
telluroglycol glycol unknown [Te],40x,.,x,0,40x
ditelluroglycol glycol unknown [Te], 40x,.,x,[Te], 40x
cyanohydrin glycol unknown C,40x, #N,x,.,x,O,40x
fluorohydrin glycol unknown F,4@x,.,x,0,4@x
chlorohydrin glycol unknown Cl,4@x,.,x,O,4@x
bromohydrin glycol unknown Br,40x,.,x,0,40x
iodohydrin glycol unknown I,4@x,.,x,0,4@x
oxide counterion oxide 0,8@x
sulfide mercaptide counterion oxide S,8@x
selenide counterion oxide [Se],8@x
```

```
telluride counterion oxide [Te],80x
methanoxymethano root methanobridge C,40x,0,x,C,40x
etheno root methanobridge C,4@x,=,x,C,4@x
metheno root metheno C,5@x
obenzeno root methanobridge c,40x,Ring,Ring1,c,40x,c,x,c,x,c,x,c,x,Ring,Ring1
epoxide enoxide counterion bridge 0,50x
episulfide counterion bridge S,5@x
sultam counterion bridge S, 40x, (=,x,0,x,), x, (=,x,0,x,), x, N, 40x
sultone sultone counterion bridge S,40x, (=,x,0,x,),x, (=,x,0,x,),x,0,40x
dicarboximide | dicarboxylicimide | dicarboxylicacidimide counterion bridge
C, 40x, (=, x, 0, x, ), x, N, x, C, 40x, =, x, 0, x
dicarboximido counterion bridge
C,40x, (=,x,0,x,),x,Ring,Ring1,.,x,C,40x,Ring,Ring2,=,x,0,x,.,x,N,40x,Ring,Ring1,
Ring, Ring2
carbolactam counterion bridge C,4@x,(=,x,0,x,),x,0,4@x
nitride counterion ionable N,12@x
phosphide counterion ionable P,12@x
antimonide counterion ionable [Sb],12@x
arsenide counterion ionable [As], 120x
hydroxide hydroxid counterion ionable 0,40x
deuteroxide deuteroxid counterion ionable 0,40x,[2H],x
hydrosulfide|hydrosulfid|sulfhydrate|sulfhydrat counterion ionable S,4@x
hydroselenide hydroselenid counterion ionable [Se], 40x
hydrotelluride hydrotellurid counterion ionable [Te], 40x
hydride hydrid counterion ionable [H], 401
deuteride deuterid counterion ionable [2H], 4@1
fluoride fluorid counterion ionable F,401
chloride chlorid muriate counterion ionable Cl, 4@1
bromide bromid counterion ionable Br, 401
iodide | iodid counterion ionable [I], 401
acetylide counterion ionable C, 40x, #[C-], x
cyanide cyanid counterion ionable C,40x, #N, x
isocyanide|isocyanid|isonitrile counterion ionable [N+],4@x,#[C-],x
cyanate cyanat counterion ionable 0,40x,C#N,x
isocyanate isocyanat counterion ionable N, 40x, =C=O, x
fulminate fulminat counterion ionable 0,40x,[N+]#[C-],x
thiocyanate|thiocyanat|sulfocyanate|sulfocyanat|sulfocyanide|sulfocyanid|rhodani
de rhodanid counterion ionable S,4@x,C#N,x
isothiocyanate|isothiocyanat|isorhodanide|isorhodanid counterion ionable
N,40x,=C=S,x
selenocyanate selenocyanat counterion ionable [Se], 40x, C#N, x
isoselenocyanate isoselenocyanat counterion ionable N,40x,=C=[Se],x
tellurocyanate tellurocyanat counterion ionable [Te], 40x, C#N, x
isotellurocyanate isotellurocyanat counterion ionable N,40x,=C=[Te],x
azide azid counterion ionable N,4@x,=[N+]=[N-],x
sulfenamide | sulfenamid counterion counterion S, 40x, N, n
sulfonazide counterion counterion S,40x,(=0)(=0)N[N+][N-],x
alcohol|icalcohol counterion counterion 0,40x
deuterol counterion counterion 0,4@x,[2H],x
selenol counterion counterion [Se], 40s
tellurol counterion counterion [Te], 40s
nitrile nitril counterion counterion N,120x
carbonitrile carbonitril counterion counterion C#N,4@x
diazonium counterion counterion [N+], 40x, #N, x
mercaptan thioalcohol counterion counterion S,40x
hydroperoxide hydroperoxid counterion ionable 0,40x,0,x
```

```
carboxaldehyde|carboxaldehyd|carboxyaldehyde|carboxyaldehyd|carbonal counterion
counterion C, 40x, (=0), x
carboxaldoxime carboxaldoxim counterion counterion C,40x,(=NO),x
carbamidine counterion counterion C,40x, (=,x,N,10n'|n2,),x,N,20n|n1
oxyfluoride counterion bridge F,40x,.,x,0,80x
oxychloride counterion bridge Cl,4@x,.,x,O,8@x
oxybromide counterion bridge Br, 40x, ., x, 0, 80x
oxviodide counterion bridge I,40x,.,x,0,80x
thiochloride counterion bridge Cl, 40x,.,x,S,80x
oxylradical counterion counterion 0,20@x
carbo carb carbeth root C,40x, (=0),x
dioxyl infix infix 0,40x,0,x
oxy infix doublebondable 0,4@x
peroxy infix doublebondable 0,40x,0,x
sulfanyl infix infix S,40x
thio infix doublebondable S,40x
mercapto infix infix S,40x
seleno infix doublebondable [Se],40x
telluro infix doublebondable [Te],40x
amino amin infix infix N, 4@n w omega
phosphino infix infix P,4@n|w|omega
phosphinyl infix infix [PH3], 40x, (=,x,0,x,),x
arsino infix infix [As], 4@n|w|omega
stibino infix infix [Sb], 4@n|w|omega
bismuthino infix infix [Bi], 4@n|w|omega
hydrazino infix infix N,2|n',N,4@1|n
hydroximino infix infix N,8@n,0,x
imino | imin infix infix N,8@n
imino imine infix N,4@n
iminio infix infix [N+],8@n
iminio imine infix [N+],4@n
nitrilo infix infix N,120n
hydrazono infix infix N,8@x,N,n
oximino infix infix N,8@x,0,0
amidosulfen infix infix S,x,N,n
sulfen infix infix S,x
sulfin infix doublebondable S,x,(=0),x
selenen infix infix [Se],x
carbonyl infix carbonyl C,40x, (=0),x
thiocarbonyl infix carbonyl C,4@x,(=S),x
selenocarbonyl infix carbonyl C,40x,(=[Se]),x
tellurocarbonyl infix carbonyl C,4@x,(=[Te]),x
thionyl infix carbonyl S,4@x,(=0),x
sulfuryl infix carbonyl S,4@x,(=0)(=0),x
carbonothioyl infix carbonyl C,40x,(=S),x
carbonimidoyl infix carbonyl C, 40x, (=N), x
carbamo | carbam infix trivial C, x, (=, x, 0, x,), x, N, n | w | omega
nitrilomethylidyne root bridge C, 40x, =, x, N, 40x
diazo azo diazo N,40x,=,x,N,x
azo infix doublebondable N, 40x, =, x, N, x
azo root bridge N,40x,=,x,N,40x
azo azo root N, x, =, x, N, x
hydrazo infix doublebondable N,x,N,4@x
hydrazo root bridge N,40x,N,40x
hydrazo azo root N,10x,N,10x
nnoazoxy azoxy infix doublebondable [N+], 40x, ([0-]), x, =, x, N, x
nnoazoxy|azoxy root bridge [N+],40x,([O-]),x,=,x,N,40x
```

azoxy azo root [N+], x, ([O-]), x, =, x, N, xazodioxy azo root [N+], x, ([O-]), x, =, x, [N+], x, [O-], xazodioxy infix doublebondable [N+], 40x, ([O-]), x, =, x, [N+], x, [O-], xazodioxy root bridge [N+], 40x, ([O-]), x, =, x, [N+], 40x, [O-], xonnazoxy | nonazoxy infix doublebondable N, 4@x, =, x, [N+], x, [O-], x diazoamino azo root N,x,=,x,N,x,N,n diazoamino root bridge N,40x,=,x,N,x,N,40n mercuri infix infix [Hg], 40x per prefix permult x,x bi prefix ringmult 2, mult ter prefix ringmult 3, mult quater prefix ringmult 4, mult quinque prefix ringmult 5, mult sexi prefix ringmult 6, mult septi prefix ringmult 7, mult octi prefix ringmult 8, mult novi prefix ringmult 9, mult deci prefix ringmult 10, mult kis prefix kis 1,x mono mon prefix prefix 1, mult hen prefix chainable 1, mult di prefix prefix 2, mult do prefix chainable 2, mult bis prefix kis 2, mult tri prefix chainable 3, mult tris prefix kis 3, mult tetr|tetra prefix chainable 4, mult pent | penta prefix chainable 5, mult hex hexa prefix chainable 6, mult hept | hepta prefix chainable 7, mult oct octa prefix chainable 8, mult non nona prefix chainable 9, mult dec deca prefix chainable 10, mult undec undeca prefix prefix 11, mult eicos eicosa icos icosa cos cosa prefix chainable 20, mult uneicos uneicosa unicos unicosa prefix prefix 21, mult triacont|triaconta|tricont|triconta prefix chainable 30, mult tetracont | tetraconta prefix chainable 40, mult pentacont pentaconta prefix chainable 50, mult hexacont hexaconta prefix chainable 60, mult heptacont | heptaconta prefix chainable 70, mult octacont|octaconta prefix chainable 80, mult nonacont nonaconta prefix chainable 90, mult hect hecta prefix chainable 100, mult dict dicta prefix chainable 200, mult trict tricta prefix chainable 300, mult tetract | tetract prefix chainable 400, mult pentact | pentacta prefix chainable 500, mult hexact hexact prefix chainable 600, mult heptact | heptacta prefix chainable 700, mult octact octacta prefix chainable 800, mult nonact|nonacta prefix chainable 900, mult kili|kilia prefix chainable 1000, mult dili dilia prefix chainable 2000, mult trili|trilia prefix chainable 3000, mult tetrali|tetralia prefix chainable 4000, mult pentali|pentalia prefix chainable 5000, mult

hexali|hexalia prefix chainable 6000, mult heptali|heptalia prefix chainable 7000, mult octali|octalia prefix chainable 8000, mult nonali|nonalia prefix chainable 9000, mult cyclo cyclo cyclo 1, cyclo spiro spiro unknown 1, spiro

onia chargegiver replacement 1, charge onium chargegiver root 1, charge onio chargegiver infix 1, charge ium | ium | ium cation chargegiver trivial 1, charge ide | ideion | ideanion chargegiver trivial -1, charge cation | ylium | ylcation suffix namedcharge 1, charge anion | ylide | ylanion suffix namedcharge -1, charge ion suffix namedcharge 0, charge

ammonium aminium root root [N+], n omega ammonio infix infix [N+], 4@n phosphonium root root [P+], x omega phosphonio infix infix [P+],40x arsonium root root [As+],x|omega arsonio infix infix [As+],40x stibonium root root [Sb+],x|omega stibonio infix infix [Sb+],40x bismuthonium root root [Bi+],x|omega bismuthonio infix infix [Bi+],40x sulfonium root root [S+],s|omega selenonium root root [Se+],s omega telluronium root root [Te+],s omega sulfoxonium root root [S+],s,=0,x sulfonio infix infix [S+],40s chloronium root root [Cl+], x omega chloronio infix infix [Cl+],40x bromonium root root [Br+], x omega bromonio infix infix [Br+],40x iodonium root root [I+],x omega iodonio infix infix [I+],40x

oxammonium root root O,x,[N+],x

actina replacement replacement [Ac], x alumina alumin replacement replacement [Al], x argenta argent replacement replacement [Ag], x arsa ars arsen replacement replacement [As], x arsora arsor replacement replacement [AsH5],x astata astat replacement replacement [At],x aura replacement replacement [Au], x aza az replacement replacement N,n bara replacement replacement [Ba], x berkela|berkel replacement replacement [Bk],x berylla|beryll replacement replacement [Be],x bisma|bism replacement replacement [Bi],x bora bor replacement replacement [B], x broma replacement replacement [Br], x cadma | cadm replacement replacement [Cd], x calca|calc replacement replacement [Ca], x californa | californ replacement replacement [Cf], x carba | carb replacement replacement [C], x

```
cera | cer replacement replacement [Ce], x
chlora replacement replacement [Cl], x
chroma|chrom replacement replacement [Cr], x
cobalta replacement replacement [Co], x
cupra cupr replacement replacement [Cu], x
cura replacement replacement [Cm], x
dysprosa dyspros replacement replacement [Dy], x
einsteina einstein replacement replacement [Es], x
europa europ replacement replacement [Eu], x
ferma|ferm replacement replacement [Fm],x
ferra|ferr replacement replacement [Fe],x
fluora replacement replacement [F], x
gadolina gadol replacement replacement [Gd], x
galla replacement replacement [Ga], x
germa|germ|german replacement replacement [Ge],x
hafna|hafn replacement replacement [Hf],x
holma | holm replacement replacement [Ho], x
inda replacement replacement [In],x
ioda replacement replacement [I], x
irida | irid replacement replacement [Ir], x
lanthana lanthan replacement replacement [La], x
lawrenca lawrenc replacement replacement [Lr], x
luteta lutet replacement replacement [Lu], x
magnesa magnes replacement replacement [Mg], x
mangana | mangan replacement replacement [Mn], x
mendeleva mendelev replacement replacement [Md], x
mercura | mercur replacement replacement [Hg], x
molybda molybd replacement replacement [Mo], x
neodyma neodym replacement replacement [Nd], x
neptuna | neptun replacement replacement [Np], x
nickela replacement replacement [Ni], x
nioba|niob replacement replacement [Nb],x
nobela nobel replacement replacement [No], x
osma osm replacement replacement [Os], x
oxa ox replacement replacement 0,x
pallada|pallad replacement replacement [Pd],x
phospha|phosph replacement replacement P,x
phosphora phosphor replacement phosphor [PH5], x
platina platin replacement replacement [Pt], x
plumba|plumb replacement replacement [Pb],x
plutona|pluton replacement replacement [Pu],x
polona polon replacement replacement [Po], x
praseodyma|praseodym replacement replacement [Pr],x
prometha prometh replacement replacement [Pm], x
protactina protactin replacement replacement [Pa], x
rada replacement replacement [Ra], x
rhena|rhen replacement replacement [Re],x
rhoda replacement replacement [Rh], x
ruthena ruthen replacement replacement [Ru], x
samara|samar replacement replacement [Sm],x
scanda | scand replacement replacement [Sc], x
selena|selen replacement replacement [Se],x
sila|sil|silic replacement replacement [Si],x
stanna|stann replacement replacement [Sn],x
stiba|stib|antimon replacement replacement [Sb],x
stibora|stibor replacement replacement [SbH5],x
stronta|stront replacement replacement [Sr],x
```

```
tantala tantal replacement replacement [Ta], x
techneta technet replacement replacement [Tc], x
tellura | tellur replacement replacement [Te], x
terba terb replacement replacement [Tb], x
thalla thall replacement replacement [T1], x
thia thi replacement replacement S,x
thora thor replacement replacement [Th], x
thula thul replacement replacement [Th], x
titana | titan replacement replacement [Ti], x
tungsta|tungst|wolframa|wolfram replacement replacement [W],x
urana uran replacement replacement [U], x
vanada | vanad replacement replacement [V], x
ytterba|ytterb replacement replacement [Yb],x
yttra yttr replacement replacement [Y], x
zinca replacement replacement [Zn],x
zircona zircon replacement replacement [2r],x
zirconyl|zirconyliv root setvalence [Zr++],x,(=0),x
vanadyliv|vanadyl root setvalence [V++],x,(=0),x
chromyl root setvalence [Cr++], x, (=0) (=0), x
uranyl root setvalence [U++],x,(=0)(=0),x
seleno selen thio unknown [Se], x
telluro tellur thio unknown [Te],x
thio thio unknown S,x
i iso tert iso 3, tert
sec tert sec 3, tert
s tert sec 4, tert
neo tert neo 4, tert
t|tert|tertiary tert tert 4,tert
imide | imid imide root N,n
imido imidyl imide root N,40n
chlorimide chlorimid imide root NCl,x
imide root oxime N,8@n
chlorimide chlorimid root oxime NC1,80x
hexafluorophosphoricacid root root [H+] \cdot [P-](F)(F)(F)(F)(F)F, x
hexafluorosilicicacid root root [H+].[H+].[Si--](F)(F)(F)(F)(F)F,x
tetrafluoroboricacid root root [H+].[B-](F)(F)(F)F,x
hexafluorozirconicicacid root root [H+].[H+].[Zr--](F)(F)(F)(F)(F)F,x
nitramin cyanic cyanic N,10x,[N+](=0)[0-],x
isocyan cyanic cyanic N,10x,=C=O,x
isothiocyan cyanic cyanic N,1@x,=C=S,x
isoselenocyan cyanic cyanic N,10x,=C=[Se],x
cyan cyanic cyanic 0,1@x,C#N,x
hydrocyan cyanic cyanic [H]C#N,x
fulmin cyanic cyanic 0,10x,[N+]#[C-],x
hydrofluor cyanic cyanic [H]F,x
hydrochlor cyanic cyanic [H]Cl,x
hydrobrom cyanic cyanic [H]Br,x
hydroiod hydriod cyanic cyanic [H]I,x
tetron cyanic cyanic 0,1,Ring,Ring1,C,2,(=0),x,C,3,C,4,(=0),x,C,5,Ring,Ring1
osm cyanic cyanic [0s](=0)(=0)(=0)=0,x
xanth|xanthogen cyanic cyanic O,x,C,x,(=,x,S,x,),x,S,s|w|omega
rhodanin cyanic cyanic
S, 1, Ring, Ring1, C, 2, (=, x, S, x,), x, N, 3, C, 4, (=, x, 0, x,), x, C, 5, Ring, Ring1
ellag cyanic cyanic 0=C30c1c(0)c(0)cc4c1c2c(0C4=0)c(0)c(0)cc23,x
```

Ī

Ō

-

13

18

Щ

ı. å

. ±

```
ur cyanic cyanic
N, 1, Ring, Ring1, C, 2, (=0), x, N, 3, C, 4, Ring, Ring2, N, 9, C, 8, (=0), x, N, 7, C, 5, =, x, Ring, Ring
g2,C,6,(=0),x,Ring,Ring1
squar quadrat cyanic cyanic
0,10x,C,x,Ring,Ring1,=,x,C,x,(,x,0,10x,),x,C,x,(=0),x,C,x,(=0),x,Ring,Ring1
crocon cyanic cyanic
0.10x, C.x, Ring, Ring1, =.x, C.x, (.x, 0.10x,), x, C.x, (=0), x, C.x, (=0), x, C.x, (=0), x, Ring
dehydroacet cyanic cyanic CC(C(C1=0)C(C=C(C)O1)=0)=0.x
ascorb|lascorbyl|lascorbyl|isoascorb pseudosugar unknown x,x
ascorb lascorb cyanic cyanic
0, x, C, 3, Ring, Ring1, [C@@H], 4, (,x, [C@@H], 5, (,x, 0, x, ), x, C, 6, 0, x, ), x, 0, x, C, 1, (=0), x,
C, 2, (, x, 0, x,), x, =, x, Ring, Ring1
ascorbyl lascorbyl root root
0,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@@H],5,(,x,0,x,),x,C,6,0,x,),x,0,x,C,1,(=0),x,
C,2,(,x,0,x,),x,=,x,Ring,Ring1
isoascorb cyanic cyanic
0,x,C,3,Ring,Ring1,[C@@H],4,(,x,[C@H],5,(,x,0,x,),x,C,6,0,x,),x,0,x,C,1,(=0),x,C
 ,2,(,x,0,x,),x,=,x,Ring,Ring1
koj cyanic cyanic
0,1,Ring,Ring1,c,2,c,3,(0),x,c,4,(=0),x,c,5,c,6,(CO),x,Ring,Ring1
picrolon cyanic cyanic 0=C1N(C2=CC=C([N+]([0-])=O)C=C2)N=C(C)C1[N+]([0-])=O,x
barbitur cyanic cyanic
N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 103, C, 4, (=, x, 0, x,), x, C, 5, C, 6, (=, x, 0, x,), x, Ri
ng, Ring1
violur cyanic cyanic
N, 101, Ring, Ring1, C, 2, (=, x, 0, x, ), x, N, 103, C, 4, (=, x, 0, x, ), x, C, 5, (=N0), x, C, 6, (=, x, 0, x
x,),x,Ring,Ring1
isobarbitur cyanic cyanic
n, 1, Ring, Ring1, c, 2, (,x,0,10x,), x, n, 3, c, 4, c, 5, (,x,0,10x,), x, c, 6, (,x,0,10x,), x, Rin
g,Ring1
cyanur cyanic cyanic
n,1,Ring,Ring1,c,2,(,x,0,1@x,),x,n,3,c,4,(,x,0,1@x,),x,n,5,c,6,(,x,0,1@x,),x,Rin
g,Ring1
isocyanur cyanic cyanic
N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 103, C, 4, (=, x, 0, x,), x, N, 105, C, 6, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, C, 2, (=, x, 0, x,), x, N, 101, Ring, Ring1, 
Ring, Ring1
melanur cyanic cyanic
n,1,Ring,Ring1,c,2,(,x,0,1@x,),x,n,3,c,4,(,x,0,1@x,),x,n,5,c,6,(,x,N,1@x,),x,Rin
q,Ring1
rhodizon cyanic cyanic
C,1,Ring,Ring1,(,x,0,10x,),x,=,x,C,2,(,x,0,10x,),x,C,3,(=0),x,C,4,(=0),x,C,5,(=0)
 ), x, C, 6, (=0), x, Ring, Ring1
chloranil cyanic cyanic
c,1,Ring,Ring1,(=0),x,c,2,(Cl),x,c,3,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,4,(=0),x,c,5,(Cl),x,c,6,(,x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c,6,(x,0,10x,),x,c
 ,0,1@x,),x,Ring,Ring1
bromanil cyanic cyanic
c, 1, Ring, Ring1, (=0), x, c, 2, (Br), x, c, 3, (,x,0,10x,), x, c, 4, (=0), x, c, 5, (Br), x, c, 6, (,x,0,10x,), x, c, 4, (=0), x, c, 5, (Br), x, c, 6, (,x,0,10x,), x, c, 6,
 ,0,10x,),x,Ring,Ring1
bromanil root root
c, 1, Ring, Ring1, (=0), x, c, 2, (Br), x, c, 3, (Br), x, c, 4, (=0), x, c, 5, (Br), x, c, 6, (Br), x, Ring
nitranil cyanic cyanic c,1,Ring,Ring1,(=0),x,c,2,([N+]([0-
 ])=0),x,c,3,(,x,0,10x,),x,c,4,(=0),x,c,5,([N+]([0-
 ])=0),x,c,6,(,x,0,10x,),x,Ring,Ring1
picr cyanic cyanic 0,1@x,c,1,Ring,Ring1,c,2,([N+]([O-])=0),x,c,3,c,4,([N+]([O-])=0)
 ) = 0), x, c, 5, c, 6, ([N+]([0-]) = 0), x, Ring, Ring 1
```

1

I

1 4

Ü

. 4

663

j

ıı de

. **.**

```
picryl root root c,4@1,Ring,Ring1,c,2,([N+]([O-])=0),x,c,3,c,4,([N+]([O-
])=0),x,c,5,c,6,([N+]([O-])=0),x,Ring,Ring1
styphn cyanic cyanic 0,10x,c,1,Ring,Ring1,c,2,([N+]([0-
]) = 0), x, c, 3, (, x, 0, 10x,), x, c, 4, ([N+]([0-]) = 0), x, c, 5, c, 6, ([N+]([0-]) = 0)
])=0),x,Ring,Ring1
pyrophosphor cyanic cyanic
P, x, (=0), x, (,x,0,10x,), x, (,x,0,10x,), x,0,x,P,x, (=0), x, (,x,0,10x,), x,0,10x
dithiopyrophosphor cyanic cyanic
P, x, (=S), x, (,x,0,10x,), x, (,x,0,10x,), x,0,x,P,x, (=S), x, (,x,0,10x,), x,0,10x
peroxydisulf cyanic cyanic
S, x, (=0) (=0), x, (,x,0,10x,), x,00,x,S,x, (=0) (=0),x,0,10x
pyrosulf cyanic cyanic S, x, (=0) (=0), x, (,x,0,10x,), x,0,x,S,x, (=0) (=0),x,0,10x
isethion cyanic cyanic 0,10x,S,x,(=0)(=0),x,C,1,C,2,0,0
hydrosulfite dithionite root root S, x, (=0), x, (,x,[0-],x,),x,S,x, (=0),x,[0-],x
dithionate root root S, x, (=0) (=0), x, (,x,[0-],x,), x, S, x, (=0) (=0), x, [0-], x
cacodyl cyanic cyanic [As](=0)(,x,0,1@x,)(C)C,x
chromotrop cyanic cyanic
c,4,Ring,Ring1,c,3,(S(=0)(=0),x,0,1@x,),x,c,2,c,1,(0),x,c,8a,Ring,Ring2,c,8,(0),
x,c,7,c,6,(S(=0)(=0),x,0,1@x,),x,c,5,c,4a,Ring,Ring1,Ring,Ring2
acid endercyanic unknown x,x
ochloranil root root
c, 1, Ring, Ring1, (=0), x, c, 2, (=0), x, c, 3, (C1), x, c, 4, (C1), x, c, 5, (C1), x, c, 6, (C1), x, Ring
q,Ring1
mchloranil root root
c,1,Ring,Ring1,(=0),x,c,2,(Cl),x,c,3,(=0),x,c,4,(Cl),x,c,5,(Cl),x,c,6,(Cl),x,Rin
pchloranil|spergon root root
g, Ring1
ate organometallicanion ate x,x
icacid oicacid acid o,80x,.,x,0,50x
ate oate acid ate 0,80x,.,x,0,50x
ic oic acid ic 0,80x,.,x,0,50x
ous acid ous 0,50x
ite acid ite 0,50x
amido acid infix 0,80x,.,x,N,50n
amido part2acid infix N,5@n
acid part2acid acid 0,50x
amide amid part2acid amide N,6@n
amide amid acid acid 0,80x,.,x,N,60n
chloramide chloramid part2acid amide N,5@n,Cl,x
bromamide|bromamid part2acid amide N,5@n,Br,x
amidine amidin imidamide acid acid N, 9@n' | n2, ., x, N, 6@n | n1
amidrazone|amidrazon acid acid N,9@n'',..,x,N,5@n|n1,N,2@n'|n2
hydrazide|hydrazid|ohydrazide|ohydrazid acid acid
0,80x,.,x,N,50n|1|n1,N,20n'|2|n2
hydrazide|hydrazid part2acid amide N,5@n|1|n1,N,2@n'|2|n2
onitrile nitrile acid nitrile N,120x
nitrile anammonide part2acid nitrile N,120x
ether part2acid acid 0,4@x,C,x,C,x
oyl acid makefree 0,80x
basic basic unknown [H],40x
aldehyde aldehyd part2acid acid H,40x
aldehyde aldehyd al acid acid 0,80x,.,x,H,40x
aldoxime aldoxim acid acid H,40x,.,x,N,80x,0,0
aldimine aldimin acid acid H, 4@x, ., x, N, 8@n
lacton | lactone part2acid lactone 0,50x
```

```
thiolacton thiolactone part2acid lactone S,50x
selenolacton | selenolactone part2acid lactone [Se],5@x
tellurolacton tellurolactone part2acid lactone [Te],5@x
lacton|lactone|olacton|olactone|iclacton|iclactone|olide|olid acid lactone
0,80x,..x,0,50x
lactam part2acid lactone N,50x
lactam olactam iclactam acid lactone 0,80x,.,x,N,50x
lactim part2acid lactone N,90x
lactim olactim iclactim acid lactone 0,40x,.,x,N,90x
sulfimide part2acid lactone N, 40x, S, 10x, (=0) (=0), x
anilide analide acid acid
0,8@x,.,x,N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
anilide analide part2acid amide
N,40n,(x,c,1',Ring,Ring1,c,2',0,c,3',m,c,4',p,c,5',c,6',Ring,Ring1,),x
anilido analido acid infix
0,8@x,.,x,N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1,),
х
anilido analido part2acid infix
N, 50n, (x, c, 1', Ring, Ring1, c, 2' | o, c, 3' | m, c, 4' | p, c, 5', c, 6', Ring, Ring1,), x
4nitroanilide pnitroanilide acid acid
O,80x,.,x,N,40n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=0)[0-
]),x,c,5',c,6',Ring,Ring1,),x
4nitroanilide pnitroanilide part2acid acid
N, 4@n, (,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=0)[0-
]),x,c,5',c,6',Ring,Ring1,),x
morpholide acid acid 0,80x,.,x,N,40x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
morpholide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
ophenone acid acid
0,80x,.,x,c,401',Ring,Ring1,c,2'|0,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
ophenone part2acid acid
c,401',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
onaphthone acid acid
0,80x,.,x,c,401',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',
c,8a',Ring,Ring1,Ring,Ring2
onaphthone part2acid acid
c,401',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',c,8a',Ring
,Ring1,Ring,Ring2
ureide acid acid 0,8@x,.,x,N,4@n,C(=0),x,N,n'
ureide part2acid amide N,4@n,C(=0),x,N,n'
piperazide acid 0,80x,.,x,N,40x,Ring,Ring1,C,x,C,x,N,x,C,x,Ring,Ring1
piperazide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperidide acid acid 0,8@x,.,x,N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
piperidide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
anhydride cyclicanhydride part2acid anhydride 0,5@x
thioanhydride part2acid anhydride S,5@x
selenoanhydride part2acid anhydride [Se],50x
telluroanhydride part2acid anhydride [Te],5@x
imid|imide part2acid anhydride N,5@x
cyclam root root S, x, (=0) (=0), x, (NC1CCCCC1), x, 0, 10x
atrop loveracid root
C,x,C,x,(,x,=,x,C,x,),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
, Ring, Ring1
pinon loveracid root CCC1CC(C(C)(C)1)C(=0)C,x
benzil loveracid root
C,x,C,a|alpha,(,x,0,x,),x,(,x,c,1,Ring,Ring1,=,x,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,
),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2
```

```
glycoll|glycol loveracid alkane C,x,C,2|w|omega,0,x
thioglycoll thioglycol loveracid root C,x,C,2,S,w omega
selenoglycoll|selenoglycol loveracid root C,x,C,2,[Se],w|omega
telluroglycoll|telluroglycol loveracid root C,x,C,2,[Te],w|omega
boro|bor|orthobor loveracid root [B],x,(,x,0,1@o'',),x,(,x,0,1@o',),x,0,1@o
metabor loveracid root [B], x, (,x,=,x,0,o',),x,0,1@o
perbor loveracid root [B], x, (, x, =, x, 0, x,) (, x, =, x, 0, x,), x, 0, 1@o
borin loveracid root [B],x,0,1@o
borono | boron loveracid counterion [B], 40x, (,x,0,100',),x,0,100
diphosphor pyrophosphor pyrophosph loveracid root
1@o''' | p2, ), x, 0, 1@o''''
dithiodiphosphor | dithiopyrophosphor | dithiopyrophosph loveracid root
1@o''' p2,),x,0,1@o'''
phosphosulf loveracid root
),x,0,1@o'''
glycerophosph alphaglycerophosph lalphaglycerophosph dalphaglycerophosph dlalpha
glycerophosph loveracid root
P,a|alpha, (=,x,0,x,)(,x,0,1@o'',)(,x,0,1@o',),x,OCC(0)CO,x
glycerophospho alphaglycerophospho lalphaglycerophospho dalphaglycerophospho dla
lphaglycerophospho loveracid root
P,4@a|alpha, (=,x,0,x,)(,x,0,1@o',),x,OCC(0)CO,x
triphosphor loveracid root
1@o''' | p2,),x,0,x,P,g | gamma,(=,x,0,x,)(,x,0,1@o'''',),x,0,1@o'''' | p3
2thiodiphosphor loveracid root
10°''' | p2,),x,0,10°'''
3thiotriphosphor loveracid root
100''' | p2, ), x, 0, x, P, g | gamma, (=, x, S, x, ) (, x, 0, 100'''', ), x, 0, 100'''' | p3
tetraphosphor loveracid root
1@o''' | p2, ), x, O, x, P, g | gamma, (=, x, O, x, ) (, x, O, 1@o'''', ), x, O, o''''' | p3, P, d | delta, (=
,x,0,x,)(,x,0,1@o''''',),x,0,1@o'''''|p4
phosphoro | phosphor | phosph | orthophosph | orthophosphor loveracid root
P, x, (=, x, 0, x, )(, x, 0, 100'', )(, x, 0, 100', ), x, 0, 100'
phosphono phosphon loveracid counterion P,40x, (=,x,0,x,) (,x,0,100',),x,0,100
phospheno phosphen loveracid root P, x, (=, x, 0, x,) (=, x, 0, x,), x, 0, 100
hypophosph loveracid root [PH0], x, (=,x,0,x,) (=,x,0,x,), x, 0, 100
phosphino phosphin loveracid root [PH2],x,(=,x,0,x,),x,0,1@o
phosphoenolpyruv loveracid root
P, x, (=, x, 0, x,) (, x, 0, 100',) (, x, 0, 100,), x, 0, x, C, x, (=C), x, C, x, (=O), x, 0, 10x
phyt loveracid root
O=P(,x,0,1@x,)(,x,0,1@x,)O[C@H]1[C@@H](OP(,x,0,1@x,)(,x,0,1@x,)=O)[C@@H](OP(,x,0,1@x,))O[C@H](OP(,x,0,1@x,)O(,x,0,1@x,))O[C@H](OP(,x,0,1@x,)O(,x,0,1@x,))O[C@H](OP(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,)O(,x,0,1@x,0,1@x,)O(,x,0,1@x,0,1@x,0,1@x,0,1@x,0,1@x,0,1@x,0,1@x,0,1@x,0,1@x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,0,1&x,
10x, 
(0x,)=0) [C@@H] (0x,0,10x,)(0,x,0,10x,)=0,x
orthoarsen|arseno|arsen loveracid root
[As], x, (=, x, 0, x, ) (, x, 0, 1@o'', ) (, x, 0, 1@o', ), x, 0, 1@o
arsenicacid root root [As],x,(=,x,0,x,)(,x,0,100'',)(,x,0,100',),x,0,100
arsino arsin loveracid root [AsH2], x, (=, x, 0, x, ), x, 0, 100
stibeno|stiben|antimon loveracid root
[Sb], x, (=, x, 0, x,) (, x, 0, 100'',) (, x, 0, 100',), x, 0, 100'
stibono|stibon loveracid counterion [Sb],4@x,(=,x,0,x,)(,x,0,1@o',),x,0,1@o
```

```
nitr loveracid root [N+], x, (,x,0,10x,)(=,x,0,x,),x,[0-],x
sulfono|sulfon loveracid counterion S,40x,(=0),x,(=0),x,0,10x
sulfino sulfin loveracid counterion S,40x,(=0),x,0,10x
sulfeno sulfen loveracid counterion S,40x,0,10x
selenono|selenon loveracid counterion [Se],4@x,(=0),x,(=0),x,0,1@x
selenino | selenin loveracid counterion [Se], 40x, (=0), x, 0, 10x
tellurono telluron loveracid counterion [Te], 40x, (=0), x, (=0), x, 0, 10x
tellurino tellurin loveracid counterion [Te], 40x, (=0), x, 0, 10x
carbox carboxyl carbo carb loveracid counterion C,4@x
carbon carbono loveracid root C,x,0,1@o
bicarbon|bicarbono loveracid root C,x,O,o,[H],x
mangan loveracid root [Mn],x, (=0)(=0),x, (,x,0,0',),x,0,1@o
permangan loveracid root [Mn],x,(=0)(=0)(=0),x,0,1@o
perrhen loveracid root [Re], x, (=0) (=0), x, 0, 1@o
perruthen loveracid root [Ru], x, (=0) (=0), x, 0, 1@0
ruthen loveracid root [Ru], x, (=0) (=0), x, (,x,0,0',),x,0,1@o
niob loveracid root [Nb], x, (=0)(=0), x, 0, 1@o
zircon loveracid root [2n], x, (=0), x, (,x,0,0',), x,0,100
tantal loveracid root [Ta], x, (=0) (=0), x, 0, 1@0
metaphosph | metaphosphor loveracid root P,x,(=0)(=0),x,0,100
bismuth loveracid root [Bi], x, (=0) (=0), x, 0, 1@0
alumin loveracid root [Al], x, (=0), x, 0, 1@o
dichrom bichrom loveracid root
[Cr], x, (=0) (=0) (,x,0,1@o',),x,0,x,[Cr],x,(=0) (=0),x,0,1@o
chrom loveracid root [Cr],x,(=0)(=0)(,x,0,1@o',),x,0,1@o
tungst|wolfram loveracid root [W], x, (=0) (=0) (,x,0,1@o',),x,0,1@o
molybd loveracid root [Mo], x, (=0) (=0) (,x,0,1@o',),x,0,1@o
silic|metasilic loveracid root [Si],x,(=0)(,x,0,1@o',),x,0,1@o
stann loveracid root [Sn], x, (=0)(,x,0,0',),x,0,1@0
titan loveracid root [Ti],x,(=,x,0,x,)(,x,0,1@o',),x,0,1@o
trifl loveracid root
S, x, (=, x, 0, x,) (, x, =0, x,) (, x, 0, 100',), x, C, x, (, x, F, x,) (, x, F, x,), x, F, x
naphthion loveracid root
S, x, (=, x, 0, x,) (, x, =0, x,) (, x, 0, 100',), x, c1ccc(N) c2ccccc12, x
sulfur | sulf loveracid root S, x, (=, x, 0, x,) (, x, =0, x,) (, x, 0, 1@o',), x, 0, 1@o'
chlorosulfamicacid root root S,x,(=0)(=0)(Cl),1@x,N,w|omega
sulfam root root S, x, (=0), x, (=0), x, (0), 10x, N, w omega
sulfamide | sulfamid root root S,x,(=0),x,(=0),x,(,x,N,1@n',),x,N,n
seleni|selen loveracid root [Se],x, (=,x,0,x,) (,x,=0,x,) (,x,0,1@0',),x,0,1@0
telluri|tellur loveracid root [Te],x,(=,x,0,x,)(,x,=0,x,)(,x,0,100',),x,0,100
sulfanil loveracid root
S, x, (=, x, 0, x,) (, x, =0, x,) (, x, 0, 1@o',), x, c, 1, Ring, Ring1, c, 2|o|ortho, c, 3|m|meta, c, 4|o|ortho, c, 3|o|ortho, c, 3|o|ortho
,(,x,N,n|n4,),x,c,5,c,6,Ring,Ring1
sulfanilamide root root
N,n|n1,S,x,(=,x,0,x,)(,x,=0,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n'|n4,),x,c,5
 ,c,6,Ring,Ring1
sulfanilamido root root
N,40x,S,x,(=,x,0,x,)(,x,=0,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n|n4,),x,c,5,c
 ,6,Ring,Ring1
sulfanilyl root root
 S,40x,(=,x,0,x,)(,x,=0,x,),x,c,1,Ring,Ring1,c,2,c,3,c,4,(,x,N,n,),x,c,5,c,6,Ring
orthanil loveracid root
S, X, (=, X, 0, X,) (, X, =0, X,) (, X, 0, 100',), X, C, 1, Ring, Ring1, C, 2, (, X, N, n,), X, C, 3, C, 4, C,
 5,c,6,Ring,Ring1
```

```
metanil loveracid root
S,x, (=,x,0,x,), (x,=0,x,), (x,0,100',),x,c,1,Ring,Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,
5,c,6,Ring,Ring1
metanilyl root root
S,40x, (=,x,0,x,), (,x,=0,x,), x,c,1,Ring,Ring1,c,2,c,3,(,x,N,n,),x,c,4,c,5,c,6,Ring
vanad metavanad loveracid root [V], x, (=,x,0,x,)(,x,=0,x,),x,0,100
orthovanad loveracid root [V], x, (=,x,0,x,)(,x,0,0'',)(,x,0,0',),x,0,100
fluor loveracid root F, x, (=, x, 0, x,) (, x, =0, x,), x, 0, 100
chlor loveracid root Cl, x, (=,x,0,x,)(,x,=0,x,),x,0,1@o
brom loveracid root Br, x, (=, x, 0, x,) (, x, =0, x,), x, 0, 100
iod loveracid root I, x, (=, x, 0, x,) (, x, =0, x,), x, 0, 100
metaperiod loveracid root I,x,(=,x,0,x,)(=,x,0,x,)(,x,=0,x,),x,0,1@o
paraperiod loveracid root
I,x, (=,x,0,x,)(,x,0,1@o''',)(,x,0,1@o'',)(,x,0,1@o'',)(,x,0,1@o',),x,0,1@o'',)
semialdehyde tailderiverdiacid acid H,40x
aldehyd deriverdiacid acid 0,80x,.,x,H,40x
am deriverdiacid acid 0,80x,.,x,N,60n
anil deriverdiacid acid
0,80x,.,x,N,40n,c,x,Ring,Ring1,c,2',c,3',c,4',c,5',c,6',Ring,Ring1
bromo brom deriveracid loveracidderiver Br,40x
chloro|chlor deriveracid loveracidderiver Cl,40x
fluoro | fluor deriveracid loveracidderiver F,40x
cyano deriveracid loveracidderiver C,4@x,#N,x
iodo | iod deriveracid loveracidderiver I,40x
amido amid deriveracid loveracidderiver N,60n
anilido deriveracid loveracidderiver
N, 4@n, c, x, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
morpholino deriveracid loveracidderiver
N,40x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
azido|azid deriveracid loveracidderiver N,4@x,=[N+]=[N-],x
bromido bromid deriveracid acid Br, 4@x
bromo brom deriveracid loveracidderiver Br,40x
chlorido chlorid deriveracid acid Cl,40x
choro chlor deriveracid loveracidderiver Cl,40x
cyanatido cyanatid deriveracid acid 0,40x,C#N,x
cyanido cyanid deriveracid acid C, 40x, #N, x
cyano deriveracid loveracidderiver C,40x, #N, x
fluorido fluorid deriveracid acid F,40x
fluoro | fluor deriveracid loveracidderiver F, 40x
hydroxam ohydroxam deriveracid acid N,5@n,0,x
hydroxim ohydroxim deriveracid acid N,8@n,0,x
hydrazon ohydrazon deriveracid acid N,8@x,N,n
iodido|iodid deriveracid acid I,40x
iodo | iod deriveracid loveracidderiver I,40x
isocyanatido isocyanatid deriveracid acid N,40x,=C=O,x
isocyanido | isocyanid deriveracid acid [N+], 40x, #[C-], x
thiocyanatido | thiocyanatid deriveracid acid S,4@x,C#N,x
isothiocyanatido | isothiocyanatid deriveracid acid N,4@x,=C=S,x
imido imid deriveracid acid N,80n
hydrazido|hydrazid deriveracid acid N,5@n|1',N,2@n'|2'
peroxo|perox|peroxy deriveracid acid 0,40x,0,1000
dithioperoxy deriveracid acid S,40x,S,10ss
seleno|selen deriveracid acid [Se],8@se
telluro tellur deriveracid acid [Te],8@te
thio|thi|thion|thiono deriveracid acid S,8@s
thiolo|thiol deriveracid acid S,5@s
```

```
per peracid peracid x,x
hypo peracid hypoacid x,x
etine|etin|etene|eten heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
oline olin olene olen heterocyc oline C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
isoxazoline|isoxazolin|isoazoline|isoazolin root oline
0,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
isothiazoline isothiazolin root oline S,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
isoselenazoline isoselenazolin root oline
[se],1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
pyrroline|pyrrolin root oline N,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
pyrazoline|pyrazolin root oline N,1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
pyrazolino root oline N,4@1,Ring,Ring1,N,2,C,3,C,4,C,5,Ring,Ring1
imidazoline | imidazolin root oline C, 2, Ring, Ring1, N, 3, C, 4, C, 5, N, 1, Ring, Ring1
sulfolene sulfolen root oline
S,1,(=,x,0,x,)(=,x,0,x,),x,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1)
sulfol root root
S, 1, (=, x, 0, x,) (=, x, 0, x,), x, Ring, Ring1, C, 2, C, 3, C, 4, C, 5, Ring, Ring1
iridine iridin heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
etidin etidine heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
olidine olidin olid heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
irene|irine|irin|iren heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
ireno|irino|irin|iren opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,Ring,Ring1
irane|iran heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,Ring,Ring1
ete|et heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
eto opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,Ring,Ring1
etane|etan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,Ring,Ring1
ole | ol heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
olo opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,Ring,Ring1
olane olan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,Ring,Ring1
ine in heterocyc ine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
ino opfuser ine c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,Ring,Ring1
inine | inin heterocyc inine
c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6,Ring,Ring1
ane an heterocyc ane
C, 1, Ring, Ring1, C, 2 o ortho, C, 3 m meta, C, 4 p para, C, 5, C, 6, Ring, Ring1
inane inan heterocyc inan
C,1,Ring,Ring1,C,2|o|ortho,C,3|m|meta,C,4|p|para,C,5,C,6,Ring,Ring1
epane epan heterocyc heterocyc C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,Ring,Ring1
epine epin heterocyc heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
epino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,Ring,Ring1
ocane ocan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,Ring,Ring1
ocine ocin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
ocino opfuser heterocyc c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,Ring,Ring1
onane onan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,Ring,Ring1
onine onin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
onino opfuser heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,Ring,Ring1
ecane ecan heterocyc heterocyc
C,1,Ring,Ring1,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,Ring,Ring1
ecine ecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
```

```
ecino ecin opfuser heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,C,9,c,10,Ring,Ring1
cyclodecine cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,Ring,Ring1
cycloundecine cycloundecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,Ring,Ring1
cyclododecine cyclododecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,Ring,Ring1
cyclotridecine cyclotridecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,Ring,Ring1
cyclotetradecine cyclotetradecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,Ring,Rin
cyclopentadecine cyclopentadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,Rin
g,Ring1
cyclohexadecine cyclohexadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6, Ring, Ring1
cycloheptadecine cycloheptadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,Ring,Ring1
cyclooctadecine cyclooctadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6,c,17,c,18,Ring,Ring1
cyclononadecine cyclononadecin heterocyc heterocyc
c,1,Ring,Ring1,c,2,c,3,c,4,c,5,c,6,c,7,c,8,c,9,c,10,c,11,c,12,c,13,c,14,c,15,c,1
6, c, 17, c, 18, c, 19, Ring, Ring1
salt salts deriv derivative salt unknown x,x
saltof salt saltof x,x
ester esters ester unknown x,x
esterswith estersof esterwith esterof ester esterwith x,x
ylene | ylen | ylenediyl ylene ylene x, x
0 roman unknown 0,x
i|1+|+1 roman unknown 1,x
ii|2+|+2 roman unknown 2,x
iii | 3+ | +3  roman unknown 3, x
iv|4+|+4 roman unknown 4,x
v|5+|+5 roman unknown 5,x
vi 6+ +6 roman unknown 6,x
vii|7+|+7 roman unknown 7,x
viii | 8+ | +8 roman unknown 8,x
ix|9+|+9 roman unknown 9,x
h hydroh unknown [H],40x
hydro root hydroroot [H], 40x
annulene annulene unknown x,x
crown crown unknown x,x
cis+trans unknown unknown x,x
vitamin unknown unknown x,x
support unknown unknown x,x
deposition unknown unknown x,x
tion | ition unknown unknown x,x
electron unknown unknown x,x
pesticide unknown unknown x,x
16n | 15n | 14n nothandled nothandled x, x
99m nothandled nothandled x,x
nonoxynol nothandled nothandled x,x
```

kiton nothandled nothandled x,x resinol nothandled nothandled x,x mersol nothandled nothandled x,x american nothandled nothandled x,x turmeric nothandled nothandled x,x phenacid|phenacide nothandled nothandled x,x sulfurized nothandled nothandled x,x branched nothandled nothandled x,x carbor nothandled nothandled x,x cuproxoline nothandled nothandled x,x dioxygenyl nothandled nothandled x,x cyclodextrin nothandled nothandled x,x octapren hexapren undecapren nothandled nothandled x,x oato ato nothandled nothandled x,x camphorato camphorate nothandled nothandled x,x acetonide nothandled nothandled x,x alcoholate nothandled nothandled x,x cyclobutoic nothandled nothandled x,x fucoidan nothandled nothandled x,x margarite nothandled nothandled x,x pyrite nothandled nothandled x,x glycerite nothandled nothandled x,x pyroxylin nothandled nothandled x,x cosmoline cosmetol nothandled nothandled x,x cupricol cuproxol nothandled nothandled x,x alol nothandled nothandled x,x prenolone nothandled nothandled x,x cergona nothandled nothandled x,x platinol nothandled nothandled x,x antin nothandled nothandled x,x germanin nothandled nothandled x,x phosphomolyb nothandled nothandled x,x anhydro nothandled nothandled x,x base nothandled nothandled x,x thioflavin thioflavine nothandled nothandled x,x dionate dionato nothandled nothandled x,x doxyl nothandled nothandled x,x acetylacetonato nothandled nothandled x,x naphtholas nothandled nothandled x,x compounded nothandled nothandled x,x ketopinic nothandled nothandled x,x indoxyl nothandled nothandled x,x indo nothandled nothandled x,x sulfobetaine nothandled nothandled x,x coenzyme nothandled nothandled x,x chlorin nothandled nothandled x,x dehydro nothandled nothandled x,x benzothiolate nothandled nothandled x,x benzanthren nothandled nothandled x,x mg nothandled nothandled x,x vinglycin nothandled nothandled x,x calanolide nothandled nothandled x,x perbor nothandled nothandled x,x dionato|dionate|acetonate nothandled nothandled x,x tetraborate nothandled nothandled x,x mefluidide nothandled nothandled x, x decavanadate nothandled nothandled x,x

```
benzin nothandled nothandled x,x
dodecin nothandled nothandled x,x
methin nothandled nothandled x,x
- nothandled nothandled x,x
tolane nothandled nothandled x,x
monocrotaline nothandled nothandled x,x
adiphenine nothandled nothandled x,x
anhydridewith nothandled nothandled x,x
terpin nothandled nothandled x,x
thiuram nothandled nothandled x,x
acaprazine nothandled unknown x,x
acaralate nothandled unknown x,x
acetazide nothandled unknown x,x
acetazolamide root root CC(NC1=NN=C(S(N)(=0)=0)S1)=O,x
acetene nothandled unknown x,x
acetohexamide nothandled unknown x,x
acetonanyl nothandled unknown x,x
aconitine nothandled unknown x,x
alipamide nothandled unknown x,x
ambrosin nothandled unknown x,x
amygdalin nothandled unknown x,x
anisene nothandled unknown x,x
anisindione nothandled unknown x,x
antichlor nothandled unknown x,x
antiethanol nothandled unknown x,x
antiformin nothandled unknown x,x
antiphen nothandled unknown x,x
arsamin nothandled unknown x,x
arsenal nothandled unknown x,x
arsenolite nothandled unknown x,x
atolide nothandled unknown x,x
azamethone nothandled unknown x,x
azinthiamide nothandled unknown x,x
azobutyl nothandled unknown x,x
azolimine nothandled unknown x,x
azopyrin nothandled unknown x,x
benzilan nothandled unknown x,x
benzilen nothandled unknown x,x
benzolene nothandled unknown x,x
benzolin nothandled unknown x,x
benzone nothandled unknown x,x
benzoxonium nothandled unknown x,x
benztropine|benzotropine root root CN3C4CC(CC3CC4)OC(C2=CC=CC=C2)C1=CC=CC=C1,x
biamine nothandled unknown x,x
bichlorendo nothandled unknown x,x
biclofibrate nothandled unknown x,x
biformylchlorazin nothandled unknown x,x
biphenate nothandled unknown x,x
bisoxyphen nothandled unknown x,x
blauramine nothandled unknown x,x
borolin nothandled unknown x,x
boroxine nothandled unknown x,x
bromacrylide nothandled unknown x,x
bromamide nothandled unknown x,x
bromethalin nothandled unknown x,x
bromhexine root root CN(C2CCCCC2)CC1=C(N)C(Br)=CC(Br)=C1,x
brominal nothandled unknown x,x
```

```
bromobutide nothandled unknown x,x
bromol nothandled unknown x,x
bromopropylate nothandled unknown x,x
bromoxanide nothandled unknown x,x
brompyrazon nothandled unknown x,x
butalamine nothandled unknown x,x
butamid nothandled unknown x,x
butethamine nothandled unknown x,x
butethanol nothandled unknown x,x
butoctamide nothandled unknown x,x
butonate nothandled unknown x,x
butone nothandled unknown x,x
butoxylate nothandled unknown x,x
butylenin nothandled unknown x,x
butylpyrin nothandled unknown x,x
calcion root root [0-]S(=0)(C1=CC(C=C(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=NC4=CC(S([0-])(=0)=0)C(N=CC(S([0-])(=0)=0)C(N=CC(S([0-])(=0)=0)C(N=CC(S([0-])(=0)=0)C(N=
]) (=0)=0)=CC5=C4C=C(0)C=C5S([0-])(=0)=0)=C30)=C3C(N=NC2=C(S([0-
) (=0) = 0) C = C6C(C(0) = CC(S([0-
camphorene nothandled unknown x,x
carbamine nothandled unknown x,x
carbamite nothandled unknown x,x
carbromal nothandled unknown x,x
carbutamide nothandled unknown x,x
carbylamine nothandled unknown x,x
cardiamid nothandled unknown x,x
cardiamine nothandled unknown x,x
cardiol nothandled unknown x,x
caryne nothandled unknown x,x
cetamid nothandled unknown x,x
chelidonine root root CN5CC1=C(C6C(CC4=CC3=C(C=C4C56)OCO3)O)C=CC2=C1OCO2, x
chinacrin chinacrine nothandled unknown x,x
chinoform nothandled unknown x,x
chinoleine nothandled unknown x,x
chloralose nothandled unknown x,x
chlorazine nothandled unknown x,x
chlorbicyclen nothandled unknown x,x
chlorbisan nothandled unknown x,x
chlorbutol nothandled unknown x,x
chlorethate nothandled unknown x,x
chlorindan nothandled unknown x,x
chlorisopropamide nothandled unknown x,x
chlormethine nothandled unknown x,x
chloroazodian nothandled unknown x,x
chlorobutin nothandled unknown x,x
chloroepoxide nothandled unknown x,x
chloronaphthine nothandled unknown x,x
chloropropamide nothandled unknown x,x
chloropropylate nothandled unknown x,x
chloropyramine root root ClC1=CC=C(C=C1)CN(C2=CC=CC=N2)CCN(C)C,x
chlorothen nothandled unknown x,x
chlorothenylpyramine nothandled unknown x,x
chlorotrisin nothandled unknown x,x
chloroxylenol nothandled unknown x,x
chlorphenamine nothandled unknown x,x
chlortalidone nothandled unknown x,x
chlorthiamid nothandled unknown x,x
```

```
chlorthioamide nothandled unknown x,x
cinchonamine nothandled unknown x,x
cineol|cineole nothandled unknown x,x
citralite nothandled unknown x,x
citrene nothandled unknown x,x
citronyl nothandled unknown x,x
citrylone nothandled unknown x,x
coniferin nothandled unknown x,x
cresotine nothandled unknown x,x
crotepoxide nothandled unknown x,x
crotonylene nothandled unknown x,x
cupricin nothandled unknown x,x
cyanogenamide nothandled unknown x,x
cyclamen nothandled unknown x,x
cyclobutyrol nothandled unknown x,x
cyclopentamine nothandled unknown x,x
cyclopentolate root root CN(CCOC(C(C2(CCCC2)0)C1=CC=CC=C1)=0)C,X
daconit nothandled unknown x,x
dazidamine nothandled unknown x,x
decitropine nothandled unknown x,x
delphinine nothandled unknown x,x
diazan nothandled unknown x,x
diazepan nothandled unknown x,x
dibrompropamidine nothandled unknown x,x
dibutin nothandled unknown x,x
dichlordiphenprop nothandled unknown x,x
dimethacrin nothandled unknown x,x
dimethoxanate nothandled unknown x,x
dimidazon nothandled unknown x,x
diodoxylin nothandled unknown x,x
dioxybenzone root root O=C(C2=CC=C(OC)C=C2O)C1=C(O)C=CC=C1,x
diphenoxylate root root
CCOC(C1(C4=CC=CC=C4)CCN(CCC(C2=CC=CC=C2)(C3=CC=CC=C3)C#N)CC1)=0,x
diphenylpyraline root root CN1CCC(OC(C3=CC=CC=C3)C2=CC=CC=C2)CC1,x
disilvn nothandled unknown x,x
disobutamide nothandled unknown x,x
dithiazanine nothandled unknown x,x
dothiepin nothandled unknown x,x
doxaminol nothandled unknown x,x
doxaprost nothandled unknown x,x
doxepin root root CN(C)CCC=C1C3=C(C=CC=C3)OCC2=C1C=CC=C2,x
doxopin nothandled unknown x,x
efuranol nothandled unknown x,x
endocet nothandled unknown x,x
endoiodin nothandled unknown x,x
esorb nothandled unknown x,x
estilben nothandled unknown x,x
ethamide nothandled unknown x,x
ethide nothandled unknown x,x
ethinamide nothandled unknown x,x
ethine nothandled unknown x,x
ethionamide root root NC(C1=CC(CC)=NC=C1)=S,x
ethoxazene nothandled unknown x,x
ethylan nothandled unknown x,x
ethylhexaldehyde nothandled unknown x,x
etryptamine nothandled unknown x,x
flavamine nothandled unknown x,x
```

```
fluoroformylone nothandled unknown x,x
fluoromethalone nothandled unknown x,x
fluorometholone nothandled unknown x,x
fluroxypyr nothandled unknown x,x
formamidoepoxide nothandled unknown x,x
formyldienolone nothandled unknown x,x
formylmethanofuran nothandled unknown x,x
fumarin nothandled unknown x,x
furalazine nothandled unknown x,x
furatoin nothandled unknown x,x
furfurin nothandled unknown x,x
gallamine nothandled unknown x,x
glucid nothandled unknown x,x
glyoxyldiureide nothandled unknown x,x
gonacrine nothandled unknown x,x
hexamethylenetetraamine nothandled unknown x,x
hexylthiocarbam nothandled unknown x,x
hydantal nothandled unknown x,x
hydantin nothandled unknown x,x
hydantoinal nothandled unknown x,x
hydantol nothandled unknown x,x
iodamide nothandled unknown x,x
iodixanol nothandled unknown x,x
iodoxamic nothandled unknown x,x
isopropalin nothandled unknown x,x
isopropamide root root CC([N+](CCC(C1=CC=CC=C1)(C2=CC=CC=C2)C(N)=0)(C(C)C)C)C,x
lactal nothandled unknown x,x
lactin nothandled unknown x,x
largon nothandled unknown x,x
laurenyne nothandled unknown x,x
laurine nothandled unknown x,x
lazo nothandled unknown x,x
lethane nothandled unknown x,x
leucol nothandled unknown x,x
lindane nothandled unknown x,x
lindol nothandled unknown x,x
lutidon nothandled unknown x.x
malonal nothandled unknown x,x
mesofolin nothandled unknown x,x
metachlorphenprop nothandled unknown x,x
methanopterin nothandled unknown x,x
methacetin nothandled unknown x,x
methacetone nothandled unknown x,x
methanofuran nothandled unknown x,x
metharsan nothandled unknown x,x
methazid nothandled unknown x,x
methazolamide root root CC(N=C1SC(S(N)(=0)=0)=NN1C)=0,x
methiodal nothandled unknown x,x
methionic nothandled unknown x,x
methoxychlor root root ClC(Cl)(Cl)C(C2=CC=C(OC)C=C2)C1=CC=C(OC)C=C1,x
methylaminopterin nothandled unknown x,x
methylenyl nothandled unknown x,x
methylone nothandled unknown x,x
monazan nothandled unknown x,x
monazol nothandled unknown x,x
monobenzone nothandled unknown x,x
montanine nothandled unknown x,x
```

```
morinamide nothandled unknown x,x
naphthonone nothandled unknown x,x
neonal nothandled unknown x,x
neophan nothandled unknown x,x
neraminol nothandled unknown x,x
nicetal nothandled unknown x,x
nicetamide nothandled unknown x,x
nitralin nothandled unknown x.x
nitrochlor nothandled unknown x,x
nitroglycerin nothandled unknown x,x
nitroglycerol nothandled unknown x,x
octatropine nothandled unknown x,x
ophthalamin nothandled unknown x,x
oxaine nothandled unknown x,x
oxamyl nothandled unknown x,x
oxanamide nothandled unknown x,x
oxanilide nothandled unknown x,x
oxanthrene nothandled unknown x,x
oxolamine root root CCN(CCC1=NC(C2=CC=CC=C2)=NO1)CC,x
oxophenarsine nothandled unknown x,x
oxoprostol nothandled unknown x,x
oxybutynin root root CCN(CC#CCOC(C(C1CCCCC1)(c2cccc2)0)=0)CC,x
oxydiazol nothandled unknown x,x
oxyfume nothandled unknown x,x
oxylan nothandled unknown x,x
oxylite nothandled unknown x,x
pentalenene nothandled unknown x,x
pentalenolactone nothandled unknown x,x
pentanochlor nothandled unknown x,x
pernitr nothandled unknown x,x
persilic nothandled unknown x,x
phenactropinium nothandled unknown x,x
phenatine nothandled unknown x,x
phenatoine nothandled unknown x,x
phenazon nothandled unknown x,x
phenformin root root N=C(NC(N)=N)NCCC1=CC=CC=C1,x
phenonyl nothandled unknown x,x
phenoxethol nothandled unknown x,x
phenoxybenzamine nothandled unknown x,x
phenoxytol nothandled unknown x,x
phenvalerate nothandled unknown x,x
phloretin root root O=C(CCC2=CC=C(0)C=C2)C1=C(0)C=C(0)C=C10, x
phosphaniline nothandled unknown x,x
phosphestrol nothandled unknown x,x
phosphotrienin nothandled unknown x,x
phthalazinol nothandled unknown x,x
phytin nothandled unknown x,x
pinacolin nothandled unknown x,x
piperazate nothandled unknown x,x
piperidolate root root O=C(OC2CN(CC)CCC2)C(C3=CC=CC=C3)C1=CC=CC=C1,x
pivalone nothandled unknown x,x
pivalyn nothandled unknown x,x
propal nothandled unknown x,x
propamidine nothandled unknown x,x
propargite nothandled unknown x,x
propazolamide nothandled unknown x,x
propiodal nothandled unknown x,x
```

propon nothandled unknown x,x proponal nothandled unknown x,x pyramin nothandled unknown x,x pyrazofurin nothandled unknown x,x pyrazolynate nothandled unknown x,x pyrazon nothandled unknown x,x pyridate nothandled unknown x,x pyridazol nothandled unknown x,x pyridenal nothandled unknown x,x pyridene nothandled unknown x,x pyrinamine nothandled unknown x,x pyroxychlor nothandled unknown x,x pyroxyfur nothandled unknown x,x razide nothandled unknown x,x razoxane nothandled unknown x,x razoxane nothandled unknown x,x razoxin nothandled unknown x,x restran nothandled unknown x,x restryl nothandled unknown x,x roxindole nothandled unknown x,x roxion nothandled unknown x,x saccharimide nothandled unknown x,x serinal nothandled unknown x,x shoxin nothandled unknown x,x silantin nothandled unknown x,x soxinol nothandled unknown x,x stoxil nothandled unknown x,x styron nothandled unknown x,x sulfacid nothandled unknown x,x sulfalene nothandled unknown x,x sulfamethazine|sulfamethazin nothandled unknown x,x sulfamethin nothandled unknown x,x sulfodiazol nothandled unknown x,x sulfurine nothandled unknown x,x sulfurol nothandled unknown x,x syncurine nothandled unknown x,x synhexyl nothandled unknown x,x synoestron nothandled unknown x,x sympren nothandled unknown x,x syringin nothandled unknown x,x talon nothandled unknown x,x tartran nothandled unknown x.x terbolan nothandled unknown x,x terbut nothandled unknown x,x terbutaline nothandled unknown x,x terbutol nothandled unknown x,x teroxalene nothandled unknown x,x tetralide nothandled unknown x,x tetralite nothandled unknown x.x tetrathiin nothandled unknown x,x thenylchlor nothandled unknown x,x thenylene nothandled unknown x,x thenylpyramine nothandled unknown x,x thiabenzazole nothandled unknown x,x thiabenzazonium nothandled unknown x,x thiadiazinol nothandled unknown x,x thiamylal root root S=C(N1)NC(C(C(C)CCC)(CC=C)C1=0)=0,x

```
thiazopyr nothandled unknown x,x
thioallate nothandled unknown x,x
thiocuran nothandled unknown x,x
thionylan nothandled unknown x,x
thioxamyl nothandled unknown x,x
thorazine nothandled unknown x,x
tolamide nothandled unknown x,x
tolamine nothandled unknown x,x
tolbutamide root root O=C(NS(C1=CC=C(C)C=C1)(=0)=0)NCCCC,x
tolcyclamide nothandled unknown x,x
tolite nothandled unknown x,x
tolnaphthate nothandled unknown x,x
tolpentamide nothandled unknown x,x
tolpropamine nothandled unknown x,x
transamine nothandled unknown x,x
triazbutyl nothandled unknown x,x
triazinate nothandled unknown x,x
tricinolon nothandled unknown x,x
tricuran nothandled unknown x,x
tropium nothandled unknown x,x
uridinal nothandled unknown x,x
ustilan nothandled unknown x,x
uval nothandled unknown x,x
uvon nothandled unknown x,x
vanillone nothandled unknown x,x
vinformide nothandled unknown x,x
vulvan nothandled unknown x,x
xanthinol nothandled unknown x,x
zded nothandled unknown x,x
zolamine nothandled unknown x,x
zoxazolamine root root NC2=NC1=CC(Cl)=CC=C102,x
trans unknown unknown x,x
alltrans unknown unknown x,x
cis unknown unknown x,x
allcis unknown unknown x,x
syn|anti unknown unknown x,x
endo unknown unknown x,x
high unknown unknown x,x
analysis analytical unknown unknown x,x
aqueous nonaqueous unknown unknown x,x
laser unknown unknown x,x
phosphoruspentoxide unknown unknown x,x
% |moll | mgml | microgml | glt | mesh | mm | cm | ml | ppm | micron | microns stopword percent x, x
0m[1m[2m[3m]4m[5m]6m[7m]8m]9m[0n]1n[2n[3n]4n[5n]6n[7n]8n]9n stopword percent x,x
ing ed stopword ing x,x
grade|purity|solution|standardsolution stopword grade x,x
7ci|8ci|9ci|10ci stopword toend x,x
aas absolute acn acs acsreagent activator aerosol amorphous analytical stopword
toend x,x
analyzer|anhydrous|approx|assay|atomic stopword toend x,x
balance|beads|bifunctional|biochemical|briquette|briquettes stopword toend x,x
capacity|chelometric|chemiluminescence|certified|chip|chips stopword toend x,x
chiral|chunk|chunks|coarse|colloidal|colorless|concentrate|contains stopword
toend x,x
crucible | crucibles | crude | crystal | crystallites | crystals | crystalline | cube stopword
toend x,x
denatured determination dispersion dry dust stopword toend x,x
```



chlorosulfamicacid buildable unknown x,x



```
each | electrolytic | electronic | electrophoresis | environmental | esterification | extrac
tion extrapure stopword toend x,x
fcc|filings|fine|finest|flake|flakes|fluorescent|fluorimetric|foil|for|freeradic
al from fume stopword toend x,x
gas|gauze|gcstandard|glacial|granular|granulate|granule|granules stopword toend
heavy|hplc|hydrophobic stopword toend x,x
indicator ingot ingots iupac stopword toend x, x
light|liquid|loose|low|lump|lumps stopword toend x,x
mainly may contain metal metals minimum moist mossy stopword toend x,x
native|natural|needle|needles|notstabilized stopword toend x,x
on|onactivatedcarbon|optical|organic stopword toend x,x
particle | pearl | pearls | pellet | pellets | photopolymerization | piece | pieces | plasticize
r stopword toend x,x
plate|plates|porous|powder|pract|practical|predominantly|predominatly|primarysta
ndard|puratronic|pure|purum stopword toend x,x
reagent | reagent for | reagentacs | redox | reference | remainder | research | ribbon | ribbons |
rod rods stopword toend x,x
scale|scales|scoop|secondarystandard|selective|sensitive|shaving|shavings|shot
stopword toend x,x
simultaneous|singlecrystal|slug|slugs|soft|solid|solution|soot|spectrographic|sp
ectrophotometric stopword toend x,x
sphere|spheres|spin|sponge|spray|stab|stabilized|stable|standard|stick|sticks|su
spension|synthetic|syrup|syrupy stopword toend x,x
tablet | tablets | tech | technical | thinfoil | titrant | topical | turnings | typically
stopword toend x,x
ultra|ultrapure|unstabilized|ultrathinfoil|usp|uvgrade stopword toend x,x
vial volumetricstandard stopword toend x,x
wet|wire|wires|wool stopword toend x,x
zonerefined stopword toend x,x
24d 245t 24dnp buildable unknown x,x
thinfoil | ultrathinfoil | singlecrystal buildable unknown x,x
antibovine | anticat | antichicken | antidog | antigoat | antiguineapig | antihorse | antihuma
n|antimonkey|antirabbit|antirat|antisheep notthisversion macromolecule x,x
tetrahydroprogesterone tetrahydroprogesteron buildable unknown x,x
hydrofluoride | hydrochloride | methochloride | methobromide | hydrobromide | hydroiodide |
hydriodide|methoiodide|methiodide|ethoiodide|ethiodide buildable unknown x,x
cyclopentadefphenanthren|cyclopentadefphenanthrene buildable unknown x,x
1011dihydrocinchon | 1011dihydrocinchonine | 1011dihydrocinchonin | 1011dihydroquinidi
ne|1011dihydrocinchonidine|1011dihydrocinchonidin buildable unknown x,x
1011dihydroquinine | 1011dihydroquinin | dihydroquinine | dihydroquinin | hydroquinine | h
ydroquinin buildable unknown x,x
alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin buildable
unknown x,x
betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
bergocryptin|bergocriptine|bergocriptin buildable unknown x,x
alphaergocryptinine alphaergocryptinin alphaergocriptinine alphaergocriptinin
buildable unknown x,x
betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
ryptinine|bergocryptinin|bergocriptinine|bergocriptinin buildable unknown x,x
1alphah5alphahtropan buildable unknown x,x
ethylvanillin|ethylcitral buildable unknown x,x
orthocatechol buildable unknown x,x
isatoicanhydride buildable unknown x,x
cresylicacid buildable unknown x,x
```

```
hexafluorophosphoricacid|hexafluorosilicicacid|hexafluorozirconicicacid|tetraflu
oroboricacid buildable unknown x,x
vlcation|vlanion buildable unknown x,x
betaalan buildable unknown x,x
crotonylalcohol buildable unknown x,x
betainealdehyde|betainaldehyd buildable unknown x,x
biotinamide|biotinamid buildable unknown x,x
angeldust buildable unknown x,x
catecholborane buildable unknown x,x
vitaminb1nitrate|thiaminenitrate|thiaminnitrate|thiaminechloride|thiaminchlorid
buildable unknown x,x
44'carbocyanine|22'carbocyanine buildable unknown x,x
vlthiol buildable unknown x,x
benzeneoxid|benzeneoxide buildable unknown x,x
card 2022cardenolide card2022enolide buildable unknown x,x
25norbornadien|25norbornadiene|2norbornene|2norbornen|5norbornene|5norbornen
buildable unknown x,x
icalcohol buildable unknown x,x
orthophthal buildable unknown x,x
neopentylglycol buildable unknown x,x
nitrogendioxide|nitricoxide|nitrousoxide buildable unknown x,x
hydrogenphosphato dihydrogenphosphato buildable unknown x,x
chloralhydrate|bromalhydrate buildable unknown x,x
vinylsulfurol buildable unknown x,x
arsenicacid buildable unknown x,x
methacr buildable unknown x,x
formamidinedisulfide buildable unknown x,x
isonitroso|isonitros|isonipecot|isobenzofuran|isocrotono|isocroton|isocrot|isoqu
inol|isochinol|qlutathionereduced buildable unknown x,x
3thiotriphosphor|2thiodiphosphor buildable unknown x,x
alphalinolen gammalinolen buildable unknown x,x
\verb|alphaglycerophosph|| lalphaglycerophosph|| dalphaglycerophosph|| dlalphaglycerophosph|| dlalphaglycerophosph||
buildable unknown x,x
alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dlalphaglycerophos
pho buildable unknown x,x
betaoestradiol|betaestradiol buildable unknown x,x
dicarboxylicimide dicarboxylicacidimide buildable unknown x,x
hydrogentartrate|hydrogenltartrate|hydrogendtartrate|lbitartrate|dbitartrate|hyd
rogenmaleate|hydrogenoxalate|hydrogensulfate|hydrogensulfite|hydrogensulfide
buildable unknown x,x
alphaionon|alphaionone|betaionone|betaionon buildable unknown x,x
sulfurdiimide sulfurdiimid buildable unknown x,x
snglycerol|snglycero|racglycerol|racglycero buildable unknown x,x
orthophosphor buildable unknown x,x
uvgrade buildable unknown x,x
ionchromatography buildable unknown x,x
dewarbenzene buildable unknown x,x
alloisoleuc|allothreono|allothreon buildable unknown x,x
anaphthoflavone|alphanaphthoflavone|bnaphthoflavone|betanaphthoflavone buildable
unknown x.x
gcstandard|primarystandard|secondarystandard buildable unknown x,x
purineriboside buildable unknown x,x
secpheneth buildable unknown x,x
4nitroanilide pnitroanilide buildable unknown x,x
betacitronell buildable unknown x,x
methylviologen|ethylviologen|benzylviologen buildable unknown x,x
 zirconyliv|vanadyliv buildable unknown x,x
```

```
activatedcarbon onactivatedcarbon buildable unknown x,x
extrapure buildable unknown x,x
maycontain buildable unknown x,x
volumetricstandard buildable unknown x,x
notstabilized buildable unknown x,x
zonerefined buildable unknown x,x
standardsolution buildable unknown x,x
wt buildable unknown x,x
phosphorustriamide buildable unknown x,x
nepsilon buildable unknown x,x
betacarboline buildable unknown x,x
pentamethylenetetramine|pentamethylenetetramin buildable unknown x,x
hexamethylenetetramine|hexamethylenetetramin buildable unknown x,x
ochloranil mchloranil pchloranil buildable unknown x,x
mesoinositol|myoinositol|dinositol|linositol|scylloinositol|epiinositol
buildable unknown x,x
stainlesssteel buildable unknown x,x
alphafuril buildable unknown x,x
alphapinene|betapinene buildable unknown x,x
chrysoidiner buildable unknown x,x
naphtholas buildable unknown x,x
neutralbuffer buildable unknown x,x
alphacumyl buildable unknown x,x
alphaphellandrene|betaphellandrene buildable unknown x,x
bisphenola buildable unknown x,x
alphalip alip buildable unknown x,x
alpharesorcyl|aresorcyl|betaresorcyl|bresorcyl|gammaresorcyl|gresorcyl|buildable
unknown x,x
gerani buildable unknown x,x
lascorb buildable unknown x,x
vitaminh|vitaminb1|thiaminedisulfide|vitaminb2|vitamine|alphatocopherol|atocophe
rol buildable unknown x,x
vitamind3 buildable unknown x,x
phenolsulfonphthalein|phenolsulfonephthalein|mcresolsulfonphthalein|mcresolsulfo
nephthalein|ocresolsulfonphthalein|ocresolsulfonephthalein|pyrocatecholsulfonpht
halein pyrocatecholsulfonephthalein pyrogallolsulfonephthalein pyrogallolsulfonep
hthalein thymolsulfonphthalein thymolsulfonephthalein phenolphthalein mcresolpht
halein ocresolphthalein pyrocatecholphthalein pyrogallolphthalein thymolphthalei
n buildable unknown x,x
freeradical buildable unknown x,x
obenzeno buildable unknown x,x
ptoluquinone | pxyloquinone buildable unknown x,x
cyclopentaaphenanthrene cyclopentaaphenanthren buildable unknown x,x
pdioxine|mdioxine|pdioxin|mdioxin buildable unknown x,x
asindacene asindacen sindacene sindacen buildable unknown x,x
sendachromeal buildable unknown x,x
isonicotino|isonicotin buildable unknown x,x
leucicacid buildable unknown x,x
isoser buildable unknown x,x
isoval buildable unknown x,x
isoleuc buildable unknown x,x
tleuc|tertleuc buildable unknown x,x
orthotyros buildable unknown x,x
mtyros metatyros buildable unknown x,x
ptyros paratyros buildable unknown x,x
hydroxyprol|3hydroxyprol|4hydroxyprol|5hydroxyprol buildable unknown x,x
3phenylalan betaphenylalan buildable unknown x,x
```

```
dtartar|dtartr|mesotartar|mesotartr buildable unknown x,x
tetrafluoroborate|tetrafluoroborate1 buildable unknown x,x
fluorosilicate | fluorosilicat | hexafluorosilicate | hexafluorosilicat buildable
unknown x,x
onnazoxy|nnoazoxy|nonazoxy buildable unknown x,x
glycolacetal|glycolketal buildable unknown x,x
moll|mgml|microqml|qlt|reagentfor|reagentacs|acsreagent buildable unknown x,x
ptosylate ptosyl buildable unknown x,x
oxazine1 oxazine4 buildable unknown x,x
tboc buildable unknown x,x
iumion|ideion|iumcation|ideanion buildable unknown x,x
isobutyro isobutyr buildable unknown x,x
isovalero isovaler buildable unknown x,x
isophthalo mphthalo isophthal mphthal buildable unknown x,x
terephthalo|pphthalo|terephthal|pphthal|buildable|unknown x,x
etherof buildable unknown x,x
esterswith estersof esterwith esterof buildable unknown x,x
saltof buildable unknown x,x
iclactone iclacton buildable unknown x,x
iclactam buildable unknown x,x
anhydridewith buildable unknown x,x
cyclicanhydride buildable unknown x,x
phosphoruspentoxide buildable unknown x,x
allcis buildable unknown x,x
alltrans buildable unknown x,x
acinitro buildable unknown x,x
astriazine|astriazin|striazine|striazin|asymtriazine|asymtriazin|symtriazine|sym
triazin buildable unknown x,x
astrioxane|astrioxan|strioxane|strioxan|asymtrioxane|asymtrioxan|symtrioxane|sym
trioxan buildable unknown x,x
astriazino|striazino|asymtriazino|symtriazino buildable unknown x,x
astrioxano|strioxano|asymtrioxano|symtrioxano buildable unknown x,x
astrithiane|astrithian|strithiane|strithian|asymtrithiane|asymtrithian|symtrithi
ane symtrithian buildable unknown x,x
thiurammonosulfide | thiuramdisulfide | thiuramtrisulfide | thiuramtrisulfid | thiuramte
trasulfide thiuramtetrasulfid buildable unknown x,x
isourea | isothiourea | 1 isoureido | 3 isoureido | 1 isothioureido | 3 isothioureido | 1 isosele
noureido | 3isoselenoureido | 1isotelluroureido | 3isotelluroureido buildable unknown
' typo typo '
" typo typo ''
± typo typo +/-
μ typo typo mu
,- typo typo -
§ typo typo beta
-> typo typo -fwdarw-
(alpha) typo typo alpha
(beta) typo typo beta
(gamma) typo typo gamma
(delta) typo typo delta
(epsilon) typo typo epsilon
(omega) typo typo omega
(ortho) typo typo ortho
(meta) typo typo meta
(para) typo typo para
(tau) typo typo tau
-oxyl typo typo -oxylradical
```

```
-thiolate typo typo -mercaptide
1-dimethylaminonaphthalene-5-sulfonyl typo typo dansyl
1,2-o-isopropylidene-d-glycer typo typo 2,3-o-isopropylidene-d-glycer
1,2-o-isopropylidene-l-glycer typo typo 2,3-o-isopropylidene-l-glycer
1,2-o-isopropylidene-glycer typo typo 2,3-o-isopropylidene-glycer
1alphah, 5alphah typo typo 1alphah5alphah
a.c.s typo typo acs
acetonamin typo typo acetonylamin
acxid typo typo acid
adonitol typo typo ribitol
aicd typo typo acid
aldazine typo typo aldehydeazine
all-e typo typo all-cis
all-z typo typo all-trans
allose typo typo alloose
allofuranose typo typo alloofuranose
allopyranose typo typo alloopyranose
alpha-tolual typo typo phenylacetal
alpha-toluat typo typo phenylacetat
alpha-toluic typo typo phenylacetic
alpha-tolunitril typo typo phenylacetonitril
aluminium typo typo aluminum
amidosulfon typo typo amidosulfur
amimo typo typo amino
ammin typo typo amin
anonan typo typo a-nonan
anonyl typo typo a-nonyl
azodicarbonamide typo typo azodicarboxamide
bathophenanthroline typo typo bathophenanthroline
benez typo typo benz
benzamin typo typo benzenamin
benzhydrazid typo typo benz-hydrazid
benzhydroxam typo typo benz-hydroxam
benzotriazoyl typo typo benzotriazolyl
bisoleam typo typo bis-oleam
bismeth typo typo dimeth
borinan typo typo bor-inan
caes typo typo ces
capro typo typo hexano
caprin typo typo decan
carboselen typo typo carboxselen
carbotellur typo typo carboxtellur
carbothi typo typo carboxthi
carboxamide typo typo carboxylamide
chinone typo typo quinone
chlorobromide typo typo chloridebromide
chlorofluoride typo typo chloridefluoride
chloroformate typo typo (chloroformate)
cinnamid typo typo cinnamamid
cis/trans typo typo cis+trans
collidin typo typo trimethylpyridin
columb typo typo niob
crotonitrile typo typo crotononitrile
dextrose typo typo d-glucose
dicaprin typo typo dicapr-in
diethylenetriaminepenta typo typo diethylenetriamine-n,n,n',n',n',-penta
diethylenetriamine-penta typo typo diethylenetriamine-n,n,n',n',n''-penta
```

:: ±

dioleate typo typo di-oleate dioleoyl typo typo di-oleoyl dionate typo typo -dionate diphosphate typo typo diphosphorate ehty typo typo ethy endo, typo typo endoerythrul typo typo glycerotetrul ethinyl typo typo ethynyl ethylenebis typo typo ethylene-bisethylenediaminetetra typo typo ethylenediamine-n,n,n',n'-tetra ethylhexoxid typo typo ethylhexanoxid etyhl typo typo ethyl exo, typo typo exoflour typo typo fluor fluoronon typo typo fluoro-non fluro typo typo fluoro furanuron typo typo furanoseuron fruct typo typo arabinohexul fucosyl typo typo fucoseyl galactosyl typo typo galactoseyl gamma-collidin typo typo 2,4,6-trimethylpyridin glucosyl typo typo glucoseyl glucuronide typo typo glucosiduronicacid guanad typo typo guanid hydrofluoren typo typo hydro-fluoren idose typo typo idoose idofuranose typo typo idoofuranose idopyranose typo typo idoopyranose imadaz typo typo imidaz imdaz typo typo imidaz inosinate typo typo inosate inosinic typo typo inosic iso- typo typo iso levulo typo typo arabinohexulo linalyl typo typo linaloyl lupetid typo typo dimethylpiperid lutid typo typo dimethylpyrid mol/l typo typo moll monocaprin typo typo monocapr-in mononitrile typo typo mono-nitrile monoole typo typo mono-ole mucic typo typo galactaric n'n' typo typo n',n' n-alpha typo typo nalpha n-(alpha) typo typo nalpha n-gamma typo typo ngamma n-delta typo typo ndelta n-omega typo typo nomega n-im- typo typo nim naphta typo typo naphtha naphthaldehyde typo typo naphthaldehyde naphthalic typo typo naphthalenedicarboxylic naphthalimid typo typo naphthalenedicarboximid naphty typo typo naphthy naphthyrid typo typo diazanaphthalene napta typo typo naphtha napth typo typo naphth

napty typo typo naphthy ocineol typo typo o-cineol oxamide typo typo oxalicamide oxeturon typo typo oxetoseuron oxiruron typo typo oxiroseuron oxylenol typo typo o-xylenol p-naphthoquinone typo typo 1,4-naphthoquinone pentacyclohexylammonium typo typo penta(cyclohexylammonium) peracet typo typo peroxyacet phath typo typo phth phenanthroline typo typo diazabenzo[a]naphthalene phosphonyl typo typo phosphonoyl phosphorin typo typo -phosphorin phosphoryl typo typo phosphoroyl phtal typo typo phthal phthaldehyde typo typo phthalaldehyde proprion typo typo propion pthal typo typo phthal psico typo typo ribohexulo pyranuron typo typo pyranoseuron rhodate typo typo rhodaate ribul typo typo erythropentul rosinate typo typo abietate s-triazol typo typo 1,2,4-triazol sacchar typo typo glucar saccharin typo typo saccharin saccharid typo typo saccharid salycyl typo typo salicyl selenious typo typo selenous septanuron typo typo septanuron siloxid typo typo silanoxid sorbo typo typo xylohexulo sorbitol typo typo glucitol stilbazol typo typo styrylpyridin sufo typo typo sulfo sulfamidic typo typo sulfamic sulfamyl typo typo sulfamoyl sulfohydrazide typo typo sulfonohydrazide sulph typo typo sulf sulphamyl typo typo sulfamoyl sulphohydrazide typo typo sulfonohydrazide tagat typo typo lyxohexul tetracarboxdiimide typo typo bis(dicarboximide) tetrahydridoborato typo typo tetrahydridoborate tetraphosphate typo typo tetraphosphorate thiazyl typo typo thiazolyl thiocarbamyl typo typo thiocarbamoyl thiol- typo typo thiolethiolan typo typo thi-olan thiolylium typo typo thiole-ylium thionochloroform typo typo chlorothionoform thiooxine typo typo thio(oxine) thiophen- typo typo thiophenethiophenamine typo typo thiophene-amine thiophenic typo typo thiopheneic thiophenone typo typo thiophene-one threonate typo typo threoonate



threonic typo typo threoonic tricaprin typo typo tricapr-in tricaproin typo typo trihexanoin trichloromethylsulfen trichloromethanesulfen typo typo (trichloromethyl)sulfen trifluoromethylsulfen trifluoromethanesulfen typo typo (trifluoromethyl)sulfen trioleate typo typo (tris)oleate triolein typo typo tri-ole-in trioleoyl typo typo (tris)oleoyl trioleyl typo typo (tris)oleyl triphosphate typo typo triphosphorate trithioperoxy typo typo thiodithioperoxy tritolyl typo typo tristolyl tropilidene typo typo 2,4,6-cyclohexatriene tyrosinate typo typo tyrosin-ate uloson typo typo ulo-on xanthylic typo typo xanthonylic xylul typo typo threopentul acidic notthisversion unknown x,x activated carbon not this version bulksolid x,x agarose notthisversion macromolecule x,x agar notthisversion macromolecule x,x agglutinin notthisversion macromolecule x,x albumin notthisversion macromolecule x,x alkonium notthisversion mixture x,x alkyl|alkyl* notthisversion mixture x,x alloy notthisversion bulksolid x,x algin notthisversion macromolecule x,x alumina notthisversion bulksolid x,x amalgam notthisversion bulksolid x,x amyloid notthisversion macromolecule x,x amylose notthis version macromolecule x, xangiotensin notthisversion macromolecule x,x anthocyanidin notthisversion mixture x,x anthocyanin notthisversion mixture x,x antibody notthisversion macromolecule x,x antibovine notthisversion macromolecule x,x anticat notthisversion macromolecule x,x antichicken notthisversion macromolecule x,x antidog notthisversion macromolecule x,x antigoat notthisversion macromolecule x,x antiquineapig notthisversion macromolecule x,x antihorse notthisversion macromolecule x,x antihuman notthisversion macromolecule x,x antimonkey notthisversion macromolecule x,x antirabbit notthisversion macromolecule x,x antirat notthisversion macromolecule x,x antisheep notthisversion macromolecule x,x ase notthisversion macromolecule x,x asphalt notthisversion mixture x,x avidin notthisversion macromolecule x,x azure notthisversion color x,x bacitracin notthisversion macromolecule x,x bead beads notthisversion bulksolid x,x bentonite notthisversion bulksolid x,x black notthisversion color x,x block notthisversion polymer x,x blue notthisversion color x,x

bombesin notthisversion macromolecule x,x bradykinin notthisversion macromolecule x,x brij notthisversion polymer x,x brilliant notthisversion color x,x bromelian notthisversion macromolecule x,x broth notthisversion mixture x,x brown notthisversion color x,x buckyball|buckyballs notthisversion fullerene x,x buffer notthisversion mixture x,x calcia notthisversion bulksolid x,x calcitonin notthisversion macromolecule x,x carborundum notthisversion bulksolid x,x carmine notthisversion color x,x carrageenan notthisversion macromolecule x,x casein notthisversion macromolecule x,x casomorphin notthisversion macromolecule x,x celite notthisversion bulksolid x,x cells notthisversion bulksolid x,x cellulose notthisversion macromolecule x,x cephalin cephalins notthisversion mixture x,x ceria notthisversion bulksolid x,x charcoal notthisversion bulksolid x,x chelate notthisversion mixture x,x chitin notthisversion macromolecule x,x chitosan notthisversion macromolecule x,x cholecystokinin notthisversion macromolecule x,x chondroitin notthisversion macromolecule x,x cocktail notthisversion mixture x,x coco notthisversion mixture x,x collagen notthisversion macromolecule x,x collodion notthisversion macromolecule x,x concanavalin notthisversion macromolecule x,x conotoxin notthisversion macromolecule x,x demi notthisversion hemi x,x detergent detergent notthisversion mixture x,x dextrin dextran notthisversion macromolecule x,x dna notthisversion macromolecule x,x dowex notthisversion polymer x,x drierite notthisversion bulksolid x,x dynorphin notthisversion macromolecule x,x edestin notthisversion macromolecule x,x endorphin notthisversion macromolecule x,x endothelin notthisversion macromolecule x,x enzyme enzymes notthisversion macromolecule x,x emulsin notthisversion macromolecule x,x extract notthisversion mixture x,x fatty notthisversion mixture x,x ferritin notthisversion macromolecule x,x fibrin notthisversion macromolecule x.x fibrinogen notthisversion macromolecule x,x fibrinolysin notthisversion macromolecule x,x fibronectin notthisversion macromolecule x,x ficin notthisversion macromolecule x,x ferrocene ferrocen notthisversion inorgcomplex x,x flavor notthisversion mixture x,x fraction notthisversion mixture x,x fullerene fullerenes notthisversion fullerene x,x

galactan notthisversion polymer x,x gelatin|gelatine notthisversion macromolecule x,x gliadin notthisversion macromolecule x,x globulin notthisversion macromolecule x,x glove|gloves notthisversion bulksolid x,x gluten notthisversion macromolecule x,x glutenin notthisversion macromolecule x,x gonadotropin notthisversion macromolecule x,x graphite notthisversion bulksolid x,x green notthisversion color x,x grey|gray notthisversion color x,x gum notthisversion mixture x,x hemi notthisversion hemi x,x hemoglobin notthisversion macromolecule x,x heparin heparan notthis version macromolecule x, x histone notthisversion macromolecule x,x hormone notthisversion macromolecule x,x hyaluron notthisversion macromolecule x,x hydrocarbon hydrocarbons notthisversion mixture x,x insulin notthisversion macromolecule x,x interferon notthisversion macromolecule x,x interleukin notthisversion macromolecule x,x inulin notthisversion macromolecule x,x isotope notthisversion isotope x,x kaolin notthisversion macromolecule x,x kephalin notthisversion macromolecule x,x keratin notthisversion macromolecule x,x kerosene kerosine notthisversion mixture x,x kit notthisversion mixture x,x kitasamycin notthisversion mixture x,x lake notthisversion color x,x laminaran notthisversion macromolecule x,x lanolin notthisversion macromolecule x,x latex notthisversion polymer x,x lecithin notthisversion macromolecule x,x lectin notthisversion macromolecule x,x lignine lignin notthis version macromolecule x,x ligroin ligroine notthis version mixture x,x litmus notthisversion macromolecule x,x lysozyme notthisversion macromolecule x,x magenta notthisversion color x,x mannan notthisversion macromolecule x,x mixed | mixt | mixture | mixtures notthisversion mixture x, x mer | mers notthisversion polymer x,x merase notthisversion macromolecule x,x mu notthisversion inorgcomplex x,x mucin notthisversion macromolecule x,x myoglobin notthisversion macromolecule x,x myosin notthisversion macromolecule x,x naphthen notthisversion macromolecule x,x neurokinin notthisversion macromolecule x,x neurotensin notthisversion macromolecule x,x nigrosine notthisversion macromolecule x,x norit notthisversion bulksolid x,x nucle notthisversion macromolecule x,x nuclein notthisversion macromolecule x,x nylon notthisversion polymer x,x



ocene ocen notthisversion inorgcomplex x,x oil notthisversion mixture x,x orange notthisversion color x,x pancreatin notthisversion macromolecule x,x papain notthisversion macromolecule x,x paraffin notthisversion bulksolid x,x paraformaldehyde notthisversion polymer x,x parathyroid notthisversion macromolecule x,x pectin notthisversion macromolecule x,x pepsin notthisversion macromolecule x,x peptide notthisversion macromolecule x,x peptone notthisversion macromolecule x,x petrol|petroleum notthisversion mixture x,x pink notthisversion color x,x pipe notthisversion bulksolid x,x pollen notthisversion bulksolid x,x poly|polymer|polymers|homopolymer notthisversion polymer x,x protamine notthisversion macromolecule x,x protein notthisversion macromolecule x,x pullulan notthisversion macromolecule x,x purple notthisversion color x,x quinhydrone notthisversion mixture x,x red notthisversion color x.x rennin notthisversion macromolecule x,x resin notthisversion polymer x,x rna notthisversion macromolecule x,x salmine notthisversion macromolecule x,x sand notthisversion bulksolid x,x saponin notthisversion macromolecule x,x scarlet notthisversion color x,x semi notthisversion hemi x,x serum notthisversion macromolecule x,x sesqui notthisversion hemi x,x sieve|sieves notthisversion bulksolid x,x silica|silicagel notthisversion bulksolid x,x somatostatin notthisversion macromolecule x,x somatotropin notthisversion macromolecule x,x stainlesssteel notthisversion bulksolid x,x starch notthisversion macromolecule x,x streptavidin notthisversion macromolecule x,x streptomycin notthisversion macromolecule x,x strip|strips notthisversion bulksolid x,x talc notthisversion bulksolid x,x tallow notthisversion mixture x,x tann notthisversion macromolecule x,x thaumatin notthisversion macromolecule x,x thoria notthisversion bulksolid x,x thrombin notthisversion macromolecule x,x titania notthisversion bulksolid x,x tragacanth notthisversion macromolecule x,x transferrin notthisversion macromolecule x,x triton notthisversion polymer x,x trypsin notthisversion macromolecule x,x tube tubes notthisversion bulksolid x,x tween notthisversion polymer x,x tylose notthisversion macromolecule x,x valve notthisversion bulksolid x,x

vasopressin notthisversion macromolecule x,x venom notthisversion mixture x,x violet notthisversion color x,x wax notthisversion bulksolid x,x white notthisversion color x,x xylan notthisversion macromolecule x,x yeast notthisversion bulksolid x,x yellow notthisversion color x,x yttria notthisversion bulksolid x,x zein notthisversion macromolecule x,x zeolite notthisversion bulksolid x,x zephiran notthisversion macromolecule x,x zephirol notthisversion macromolecule x,x zirconia notthisversion bulksolid x,x zyme notthisversion macromolecule x,x ortho ordinal ordinal x,x epsilon ordinal ordinal x,x nepsilon ordinal ordinal x,x npi ordinal ordinal x,x